



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 06:42 am BST

PDB ID : 4QII  
Title : Crystal Structure of type II MenB from Mycobacteria tuberculosis  
Authors : Song, H.G.; Tse, Y.S.; Sung, H.P.; Guo, Z.H.  
Deposited on : 2014-05-31  
Resolution : 1.64 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](mailto: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.

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

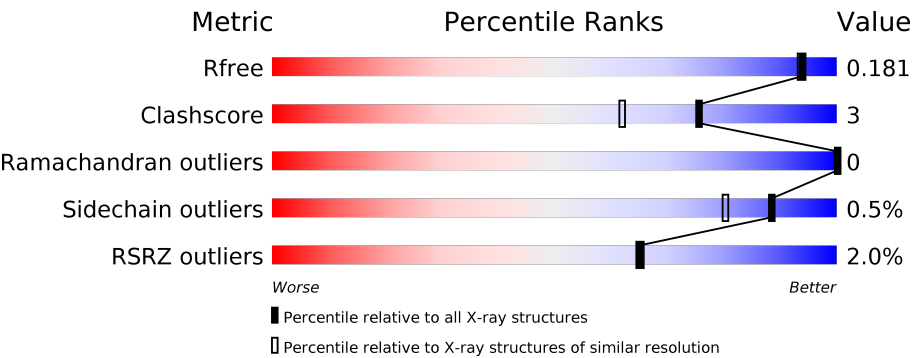
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 1.64 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	334	<div><div>3%</div><div><div></div><div>84%</div><div>6%</div><div>10%</div></div></div>
1	B	334	<div><div>2%</div><div><div></div><div>86%</div><div>•</div><div>10%</div></div></div>
1	C	334	<div><div>%</div><div><div></div><div>85%</div><div>5%</div><div>10%</div></div></div>
1	D	334	<div><div>%</div><div><div></div><div>85%</div><div>•</div><div>10%</div></div></div>
1	E	334	<div><div>%</div><div><div></div><div>85%</div><div>•</div><div>11%</div></div></div>
1	F	334	<div><div>%</div><div><div></div><div>85%</div><div>•</div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	334	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>86%</div><div>10%</div></div><div></div></div>
1	H	334	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>86%</div><div>10%</div></div><div></div></div>
1	I	334	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>86%</div><div>10%</div></div><div></div></div>
1	J	334	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>85%</div><div>11%</div></div><div></div></div>
1	K	334	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>85%</div><div>11%</div></div><div></div></div>
1	L	334	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>86%</div><div>11%</div></div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32663 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 1,4-Dihydroxy-2-naphthoyl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2341	1474	423	435	9			
1	B	301	Total	C	N	O	S	0	0	0
			2352	1482	425	436	9			
1	C	301	Total	C	N	O	S	0	0	0
			2345	1478	424	434	9			
1	D	299	Total	C	N	O	S	0	0	0
			2336	1470	425	432	9			
1	E	298	Total	C	N	O	S	0	0	0
			2331	1469	425	428	9			
1	F	298	Total	C	N	O	S	0	0	0
			2338	1472	425	432	9			
1	G	301	Total	C	N	O	S	0	0	0
			2350	1480	425	436	9			
1	H	301	Total	C	N	O	S	0	0	0
			2349	1481	425	434	9			
1	I	301	Total	C	N	O	S	0	0	0
			2352	1482	425	436	9			
1	J	297	Total	C	N	O	S	0	0	0
			2319	1461	420	429	9			
1	K	298	Total	C	N	O	S	0	0	0
			2337	1471	425	432	9			
1	L	298	Total	C	N	O	S	0	0	0
			2333	1470	422	432	9			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P9WNP5
A	-18	GLY	-	EXPRESSION TAG	UNP P9WNP5
A	-17	SER	-	EXPRESSION TAG	UNP P9WNP5
A	-16	SER	-	EXPRESSION TAG	UNP P9WNP5
A	-15	HIS	-	EXPRESSION TAG	UNP P9WNP5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	EXPRESSION TAG	UNP P9WNP5
A	-13	HIS	-	EXPRESSION TAG	UNP P9WNP5
A	-12	HIS	-	EXPRESSION TAG	UNP P9WNP5
A	-11	HIS	-	EXPRESSION TAG	UNP P9WNP5
A	-10	HIS	-	EXPRESSION TAG	UNP P9WNP5
A	-9	SER	-	EXPRESSION TAG	UNP P9WNP5
A	-8	SER	-	EXPRESSION TAG	UNP P9WNP5
A	-7	GLY	-	EXPRESSION TAG	UNP P9WNP5
A	-6	LEU	-	EXPRESSION TAG	UNP P9WNP5
A	-5	VAL	-	EXPRESSION TAG	UNP P9WNP5
A	-4	PRO	-	EXPRESSION TAG	UNP P9WNP5
A	-3	ARG	-	EXPRESSION TAG	UNP P9WNP5
A	-2	GLY	-	EXPRESSION TAG	UNP P9WNP5
A	-1	SER	-	EXPRESSION TAG	UNP P9WNP5
A	0	HIS	-	EXPRESSION TAG	UNP P9WNP5
B	-19	MET	-	EXPRESSION TAG	UNP P9WNP5
B	-18	GLY	-	EXPRESSION TAG	UNP P9WNP5
B	-17	SER	-	EXPRESSION TAG	UNP P9WNP5
B	-16	SER	-	EXPRESSION TAG	UNP P9WNP5
B	-15	HIS	-	EXPRESSION TAG	UNP P9WNP5
B	-14	HIS	-	EXPRESSION TAG	UNP P9WNP5
B	-13	HIS	-	EXPRESSION TAG	UNP P9WNP5
B	-12	HIS	-	EXPRESSION TAG	UNP P9WNP5
B	-11	HIS	-	EXPRESSION TAG	UNP P9WNP5
B	-10	HIS	-	EXPRESSION TAG	UNP P9WNP5
B	-9	SER	-	EXPRESSION TAG	UNP P9WNP5
B	-8	SER	-	EXPRESSION TAG	UNP P9WNP5
B	-7	GLY	-	EXPRESSION TAG	UNP P9WNP5
B	-6	LEU	-	EXPRESSION TAG	UNP P9WNP5
B	-5	VAL	-	EXPRESSION TAG	UNP P9WNP5
B	-4	PRO	-	EXPRESSION TAG	UNP P9WNP5
B	-3	ARG	-	EXPRESSION TAG	UNP P9WNP5
B	-2	GLY	-	EXPRESSION TAG	UNP P9WNP5
B	-1	SER	-	EXPRESSION TAG	UNP P9WNP5
B	0	HIS	-	EXPRESSION TAG	UNP P9WNP5
C	-19	MET	-	EXPRESSION TAG	UNP P9WNP5
C	-18	GLY	-	EXPRESSION TAG	UNP P9WNP5
C	-17	SER	-	EXPRESSION TAG	UNP P9WNP5
C	-16	SER	-	EXPRESSION TAG	UNP P9WNP5
C	-15	HIS	-	EXPRESSION TAG	UNP P9WNP5
C	-14	HIS	-	EXPRESSION TAG	UNP P9WNP5
C	-13	HIS	-	EXPRESSION TAG	UNP P9WNP5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	EXPRESSION TAG	UNP P9WNP5
C	-11	HIS	-	EXPRESSION TAG	UNP P9WNP5
C	-10	HIS	-	EXPRESSION TAG	UNP P9WNP5
C	-9	SER	-	EXPRESSION TAG	UNP P9WNP5
C	-8	SER	-	EXPRESSION TAG	UNP P9WNP5
C	-7	GLY	-	EXPRESSION TAG	UNP P9WNP5
C	-6	LEU	-	EXPRESSION TAG	UNP P9WNP5
C	-5	VAL	-	EXPRESSION TAG	UNP P9WNP5
C	-4	PRO	-	EXPRESSION TAG	UNP P9WNP5
C	-3	ARG	-	EXPRESSION TAG	UNP P9WNP5
C	-2	GLY	-	EXPRESSION TAG	UNP P9WNP5
C	-1	SER	-	EXPRESSION TAG	UNP P9WNP5
C	0	HIS	-	EXPRESSION TAG	UNP P9WNP5
D	-19	MET	-	EXPRESSION TAG	UNP P9WNP5
D	-18	GLY	-	EXPRESSION TAG	UNP P9WNP5
D	-17	SER	-	EXPRESSION TAG	UNP P9WNP5
D	-16	SER	-	EXPRESSION TAG	UNP P9WNP5
D	-15	HIS	-	EXPRESSION TAG	UNP P9WNP5
D	-14	HIS	-	EXPRESSION TAG	UNP P9WNP5
D	-13	HIS	-	EXPRESSION TAG	UNP P9WNP5
D	-12	HIS	-	EXPRESSION TAG	UNP P9WNP5
D	-11	HIS	-	EXPRESSION TAG	UNP P9WNP5
D	-10	HIS	-	EXPRESSION TAG	UNP P9WNP5
D	-9	SER	-	EXPRESSION TAG	UNP P9WNP5
D	-8	SER	-	EXPRESSION TAG	UNP P9WNP5
D	-7	GLY	-	EXPRESSION TAG	UNP P9WNP5
D	-6	LEU	-	EXPRESSION TAG	UNP P9WNP5
D	-5	VAL	-	EXPRESSION TAG	UNP P9WNP5
D	-4	PRO	-	EXPRESSION TAG	UNP P9WNP5
D	-3	ARG	-	EXPRESSION TAG	UNP P9WNP5
D	-2	GLY	-	EXPRESSION TAG	UNP P9WNP5
D	-1	SER	-	EXPRESSION TAG	UNP P9WNP5
D	0	HIS	-	EXPRESSION TAG	UNP P9WNP5
E	-19	MET	-	EXPRESSION TAG	UNP P9WNP5
E	-18	GLY	-	EXPRESSION TAG	UNP P9WNP5
E	-17	SER	-	EXPRESSION TAG	UNP P9WNP5
E	-16	SER	-	EXPRESSION TAG	UNP P9WNP5
E	-15	HIS	-	EXPRESSION TAG	UNP P9WNP5
E	-14	HIS	-	EXPRESSION TAG	UNP P9WNP5
E	-13	HIS	-	EXPRESSION TAG	UNP P9WNP5
E	-12	HIS	-	EXPRESSION TAG	UNP P9WNP5
E	-11	HIS	-	EXPRESSION TAG	UNP P9WNP5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	EXPRESSION TAG	UNP P9WNP5
E	-9	SER	-	EXPRESSION TAG	UNP P9WNP5
E	-8	SER	-	EXPRESSION TAG	UNP P9WNP5
E	-7	GLY	-	EXPRESSION TAG	UNP P9WNP5
E	-6	LEU	-	EXPRESSION TAG	UNP P9WNP5
E	-5	VAL	-	EXPRESSION TAG	UNP P9WNP5
E	-4	PRO	-	EXPRESSION TAG	UNP P9WNP5
E	-3	ARG	-	EXPRESSION TAG	UNP P9WNP5
E	-2	GLY	-	EXPRESSION TAG	UNP P9WNP5
E	-1	SER	-	EXPRESSION TAG	UNP P9WNP5
E	0	HIS	-	EXPRESSION TAG	UNP P9WNP5
F	-19	MET	-	EXPRESSION TAG	UNP P9WNP5
F	-18	GLY	-	EXPRESSION TAG	UNP P9WNP5
F	-17	SER	-	EXPRESSION TAG	UNP P9WNP5
F	-16	SER	-	EXPRESSION TAG	UNP P9WNP5
F	-15	HIS	-	EXPRESSION TAG	UNP P9WNP5
F	-14	HIS	-	EXPRESSION TAG	UNP P9WNP5
F	-13	HIS	-	EXPRESSION TAG	UNP P9WNP5
F	-12	HIS	-	EXPRESSION TAG	UNP P9WNP5
F	-11	HIS	-	EXPRESSION TAG	UNP P9WNP5
F	-10	HIS	-	EXPRESSION TAG	UNP P9WNP5
F	-9	SER	-	EXPRESSION TAG	UNP P9WNP5
F	-8	SER	-	EXPRESSION TAG	UNP P9WNP5
F	-7	GLY	-	EXPRESSION TAG	UNP P9WNP5
F	-6	LEU	-	EXPRESSION TAG	UNP P9WNP5
F	-5	VAL	-	EXPRESSION TAG	UNP P9WNP5
F	-4	PRO	-	EXPRESSION TAG	UNP P9WNP5
F	-3	ARG	-	EXPRESSION TAG	UNP P9WNP5
F	-2	GLY	-	EXPRESSION TAG	UNP P9WNP5
F	-1	SER	-	EXPRESSION TAG	UNP P9WNP5
F	0	HIS	-	EXPRESSION TAG	UNP P9WNP5
G	-19	MET	-	EXPRESSION TAG	UNP P9WNP5
G	-18	GLY	-	EXPRESSION TAG	UNP P9WNP5
G	-17	SER	-	EXPRESSION TAG	UNP P9WNP5
G	-16	SER	-	EXPRESSION TAG	UNP P9WNP5
G	-15	HIS	-	EXPRESSION TAG	UNP P9WNP5
G	-14	HIS	-	EXPRESSION TAG	UNP P9WNP5
G	-13	HIS	-	EXPRESSION TAG	UNP P9WNP5
G	-12	HIS	-	EXPRESSION TAG	UNP P9WNP5
G	-11	HIS	-	EXPRESSION TAG	UNP P9WNP5
G	-10	HIS	-	EXPRESSION TAG	UNP P9WNP5
G	-9	SER	-	EXPRESSION TAG	UNP P9WNP5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	SER	-	EXPRESSION TAG	UNP P9WNP5
G	-7	GLY	-	EXPRESSION TAG	UNP P9WNP5
G	-6	LEU	-	EXPRESSION TAG	UNP P9WNP5
G	-5	VAL	-	EXPRESSION TAG	UNP P9WNP5
G	-4	PRO	-	EXPRESSION TAG	UNP P9WNP5
G	-3	ARG	-	EXPRESSION TAG	UNP P9WNP5
G	-2	GLY	-	EXPRESSION TAG	UNP P9WNP5
G	-1	SER	-	EXPRESSION TAG	UNP P9WNP5
G	0	HIS	-	EXPRESSION TAG	UNP P9WNP5
H	-19	MET	-	EXPRESSION TAG	UNP P9WNP5
H	-18	GLY	-	EXPRESSION TAG	UNP P9WNP5
H	-17	SER	-	EXPRESSION TAG	UNP P9WNP5
H	-16	SER	-	EXPRESSION TAG	UNP P9WNP5
H	-15	HIS	-	EXPRESSION TAG	UNP P9WNP5
H	-14	HIS	-	EXPRESSION TAG	UNP P9WNP5
H	-13	HIS	-	EXPRESSION TAG	UNP P9WNP5
H	-12	HIS	-	EXPRESSION TAG	UNP P9WNP5
H	-11	HIS	-	EXPRESSION TAG	UNP P9WNP5
H	-10	HIS	-	EXPRESSION TAG	UNP P9WNP5
H	-9	SER	-	EXPRESSION TAG	UNP P9WNP5
H	-8	SER	-	EXPRESSION TAG	UNP P9WNP5
H	-7	GLY	-	EXPRESSION TAG	UNP P9WNP5
H	-6	LEU	-	EXPRESSION TAG	UNP P9WNP5
H	-5	VAL	-	EXPRESSION TAG	UNP P9WNP5
H	-4	PRO	-	EXPRESSION TAG	UNP P9WNP5
H	-3	ARG	-	EXPRESSION TAG	UNP P9WNP5
H	-2	GLY	-	EXPRESSION TAG	UNP P9WNP5
H	-1	SER	-	EXPRESSION TAG	UNP P9WNP5
H	0	HIS	-	EXPRESSION TAG	UNP P9WNP5
I	-19	MET	-	EXPRESSION TAG	UNP P9WNP5
I	-18	GLY	-	EXPRESSION TAG	UNP P9WNP5
I	-17	SER	-	EXPRESSION TAG	UNP P9WNP5
I	-16	SER	-	EXPRESSION TAG	UNP P9WNP5
I	-15	HIS	-	EXPRESSION TAG	UNP P9WNP5
I	-14	HIS	-	EXPRESSION TAG	UNP P9WNP5
I	-13	HIS	-	EXPRESSION TAG	UNP P9WNP5
I	-12	HIS	-	EXPRESSION TAG	UNP P9WNP5
I	-11	HIS	-	EXPRESSION TAG	UNP P9WNP5
I	-10	HIS	-	EXPRESSION TAG	UNP P9WNP5
I	-9	SER	-	EXPRESSION TAG	UNP P9WNP5
I	-8	SER	-	EXPRESSION TAG	UNP P9WNP5
I	-7	GLY	-	EXPRESSION TAG	UNP P9WNP5

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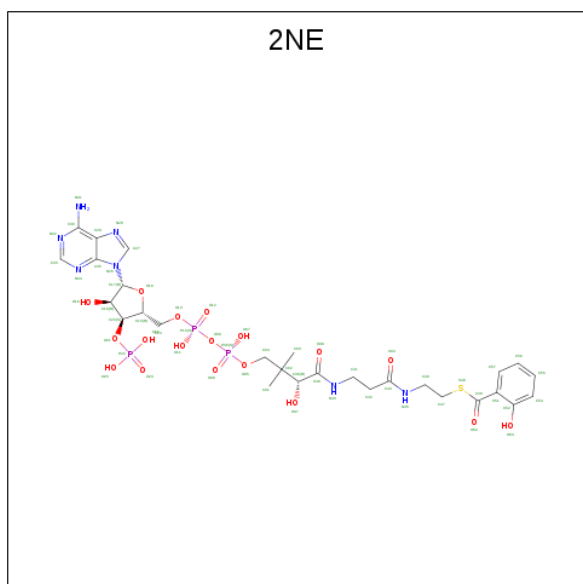
Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	EXPRESSION TAG	UNP P9WNP5
I	-5	VAL	-	EXPRESSION TAG	UNP P9WNP5
I	-4	PRO	-	EXPRESSION TAG	UNP P9WNP5
I	-3	ARG	-	EXPRESSION TAG	UNP P9WNP5
I	-2	GLY	-	EXPRESSION TAG	UNP P9WNP5
I	-1	SER	-	EXPRESSION TAG	UNP P9WNP5
I	0	HIS	-	EXPRESSION TAG	UNP P9WNP5
J	-19	MET	-	EXPRESSION TAG	UNP P9WNP5
J	-18	GLY	-	EXPRESSION TAG	UNP P9WNP5
J	-17	SER	-	EXPRESSION TAG	UNP P9WNP5
J	-16	SER	-	EXPRESSION TAG	UNP P9WNP5
J	-15	HIS	-	EXPRESSION TAG	UNP P9WNP5
J	-14	HIS	-	EXPRESSION TAG	UNP P9WNP5
J	-13	HIS	-	EXPRESSION TAG	UNP P9WNP5
J	-12	HIS	-	EXPRESSION TAG	UNP P9WNP5
J	-11	HIS	-	EXPRESSION TAG	UNP P9WNP5
J	-10	HIS	-	EXPRESSION TAG	UNP P9WNP5
J	-9	SER	-	EXPRESSION TAG	UNP P9WNP5
J	-8	SER	-	EXPRESSION TAG	UNP P9WNP5
J	-7	GLY	-	EXPRESSION TAG	UNP P9WNP5
J	-6	LEU	-	EXPRESSION TAG	UNP P9WNP5
J	-5	VAL	-	EXPRESSION TAG	UNP P9WNP5
J	-4	PRO	-	EXPRESSION TAG	UNP P9WNP5
J	-3	ARG	-	EXPRESSION TAG	UNP P9WNP5
J	-2	GLY	-	EXPRESSION TAG	UNP P9WNP5
J	-1	SER	-	EXPRESSION TAG	UNP P9WNP5
J	0	HIS	-	EXPRESSION TAG	UNP P9WNP5
K	-19	MET	-	EXPRESSION TAG	UNP P9WNP5
K	-18	GLY	-	EXPRESSION TAG	UNP P9WNP5
K	-17	SER	-	EXPRESSION TAG	UNP P9WNP5
K	-16	SER	-	EXPRESSION TAG	UNP P9WNP5
K	-15	HIS	-	EXPRESSION TAG	UNP P9WNP5
K	-14	HIS	-	EXPRESSION TAG	UNP P9WNP5
K	-13	HIS	-	EXPRESSION TAG	UNP P9WNP5
K	-12	HIS	-	EXPRESSION TAG	UNP P9WNP5
K	-11	HIS	-	EXPRESSION TAG	UNP P9WNP5
K	-10	HIS	-	EXPRESSION TAG	UNP P9WNP5
K	-9	SER	-	EXPRESSION TAG	UNP P9WNP5
K	-8	SER	-	EXPRESSION TAG	UNP P9WNP5
K	-7	GLY	-	EXPRESSION TAG	UNP P9WNP5
K	-6	LEU	-	EXPRESSION TAG	UNP P9WNP5
K	-5	VAL	-	EXPRESSION TAG	UNP P9WNP5

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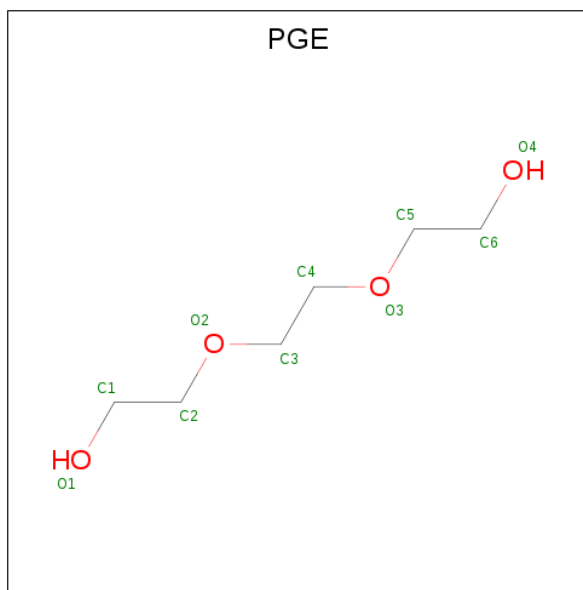
Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	EXPRESSION TAG	UNP P9WNP5
K	-3	ARG	-	EXPRESSION TAG	UNP P9WNP5
K	-2	GLY	-	EXPRESSION TAG	UNP P9WNP5
K	-1	SER	-	EXPRESSION TAG	UNP P9WNP5
K	0	HIS	-	EXPRESSION TAG	UNP P9WNP5
L	-19	MET	-	EXPRESSION TAG	UNP P9WNP5
L	-18	GLY	-	EXPRESSION TAG	UNP P9WNP5
L	-17	SER	-	EXPRESSION TAG	UNP P9WNP5
L	-16	SER	-	EXPRESSION TAG	UNP P9WNP5
L	-15	HIS	-	EXPRESSION TAG	UNP P9WNP5
L	-14	HIS	-	EXPRESSION TAG	UNP P9WNP5
L	-13	HIS	-	EXPRESSION TAG	UNP P9WNP5
L	-12	HIS	-	EXPRESSION TAG	UNP P9WNP5
L	-11	HIS	-	EXPRESSION TAG	UNP P9WNP5
L	-10	HIS	-	EXPRESSION TAG	UNP P9WNP5
L	-9	SER	-	EXPRESSION TAG	UNP P9WNP5
L	-8	SER	-	EXPRESSION TAG	UNP P9WNP5
L	-7	GLY	-	EXPRESSION TAG	UNP P9WNP5
L	-6	LEU	-	EXPRESSION TAG	UNP P9WNP5
L	-5	VAL	-	EXPRESSION TAG	UNP P9WNP5
L	-4	PRO	-	EXPRESSION TAG	UNP P9WNP5
L	-3	ARG	-	EXPRESSION TAG	UNP P9WNP5
L	-2	GLY	-	EXPRESSION TAG	UNP P9WNP5
L	-1	SER	-	EXPRESSION TAG	UNP P9WNP5
L	0	HIS	-	EXPRESSION TAG	UNP P9WNP5

- Molecule 2 is Salicylyl CoA (three-letter code: 2NE) (formula:  $C_{28}H_{40}N_7O_{18}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	K	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 10 6 4	0	0
3	D	1	Total C O 10 6 4	0	0
3	G	1	Total C O 10 6 4	0	0
3	J	1	Total C O 10 6 4	0	0

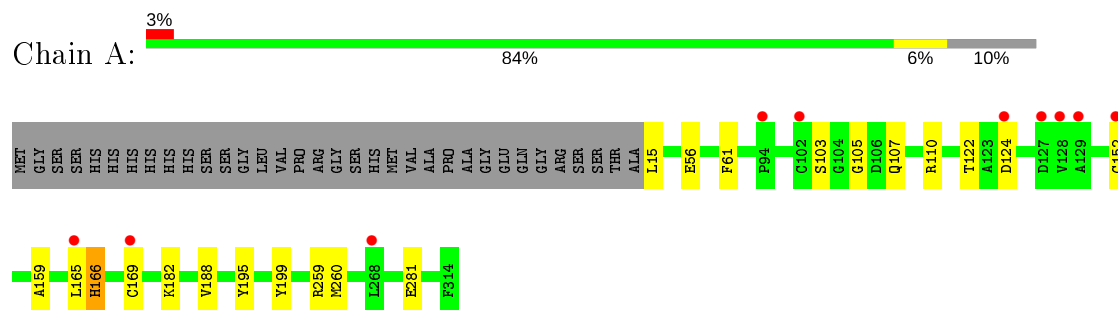
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	349	Total O 349 349	0	0
4	B	325	Total O 325 325	0	0
4	C	326	Total O 326 326	0	0
4	D	296	Total O 296 296	0	0
4	E	331	Total O 331 331	0	0
4	F	347	Total O 347 347	0	0
4	G	366	Total O 366 366	0	0
4	H	330	Total O 330 330	0	0
4	I	344	Total O 344 344	0	0
4	J	266	Total O 266 266	0	0
4	K	281	Total O 281 281	0	0
4	L	295	Total O 295 295	0	0

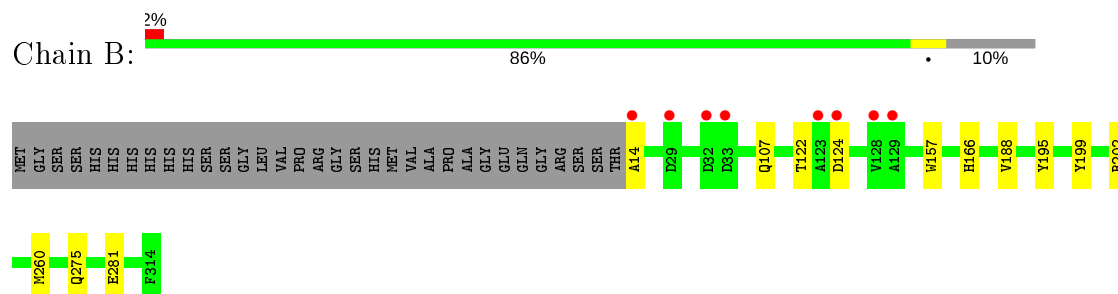
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

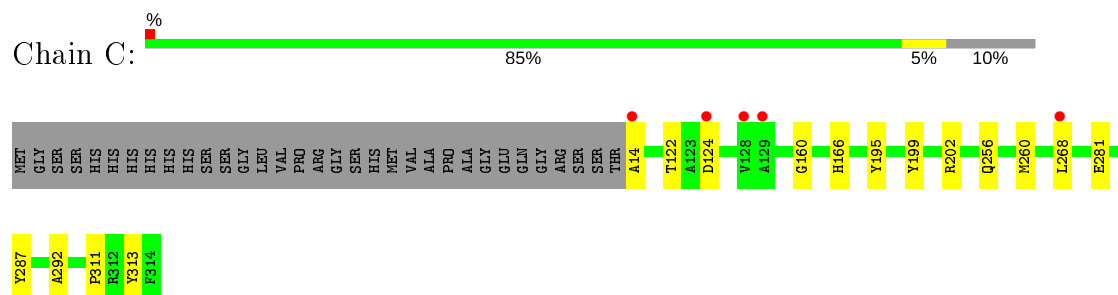
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



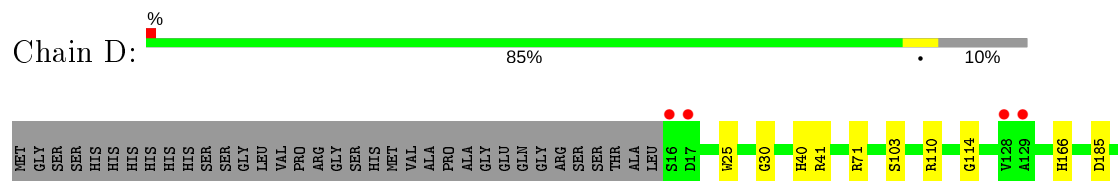
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase

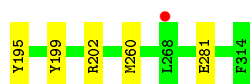


- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase

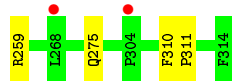
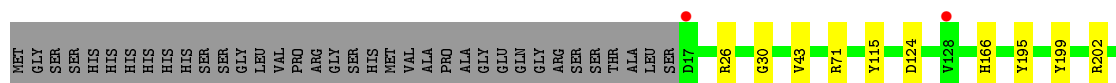
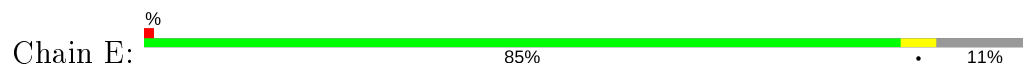


- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase

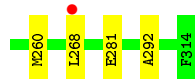
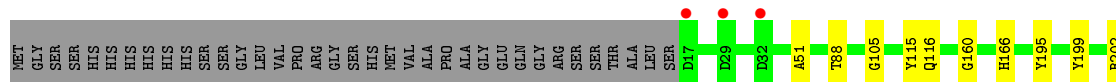
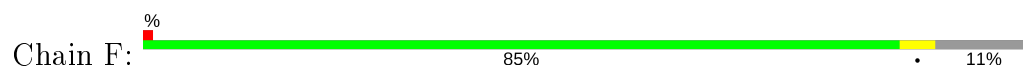




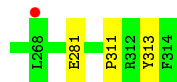
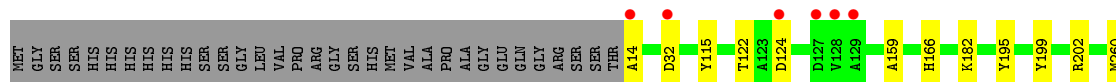
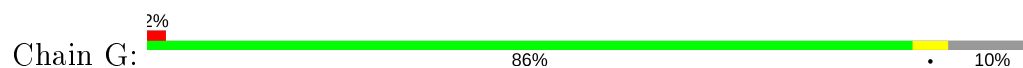
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



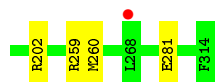
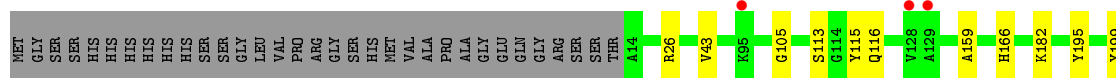
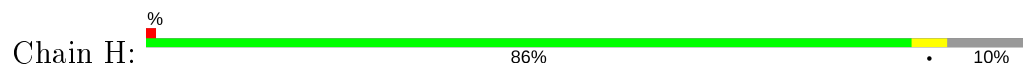
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



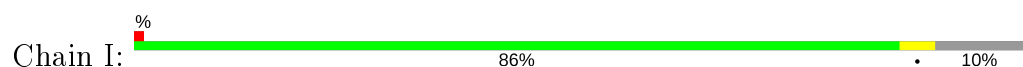
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase

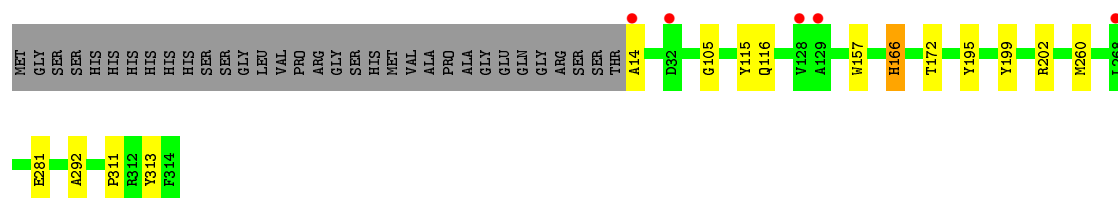


- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase

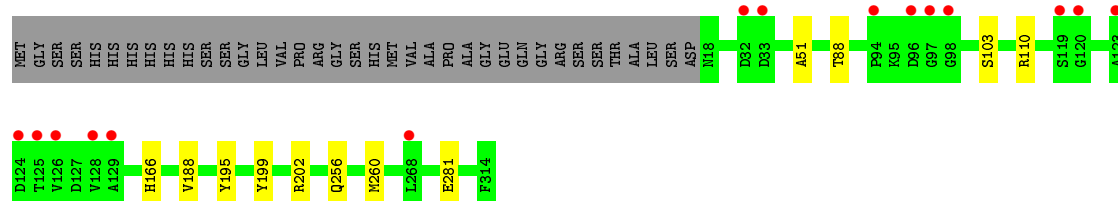
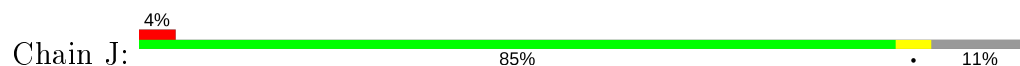


- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase

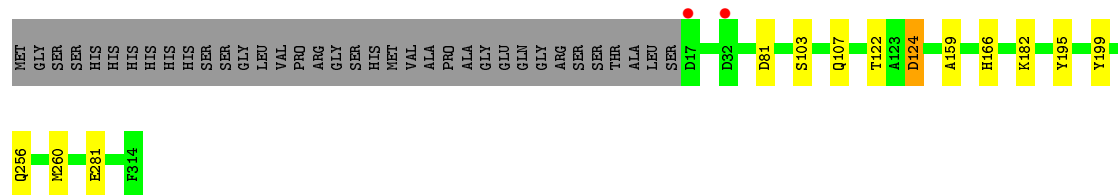
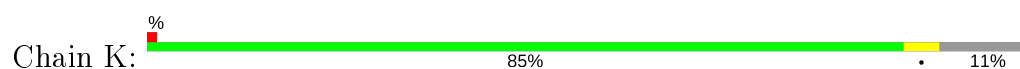




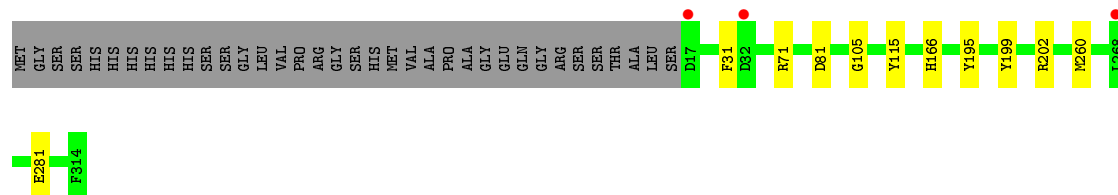
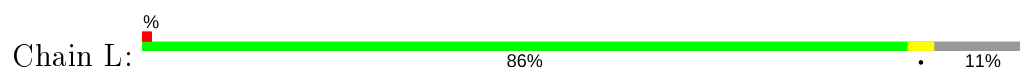
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.47Å 147.72Å 140.82Å 90.00° 103.45° 90.00°	Depositor
Resolution (Å)	34.95 – 1.64 34.96 – 1.64	Depositor EDS
% Data completeness (in resolution range)	99.1 (34.95-1.64) 94.1 (34.96-1.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 1.64Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.151 , 0.181 0.153 , 0.181	Depositor DCC
$R_{free}$ test set	22034 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	32663	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, 2NE

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	0.35	0/2398	0.54	0/3253
1	B	0.35	0/2409	0.53	0/3266
1	C	0.34	0/2402	0.52	0/3258
1	D	0.33	0/2393	0.51	0/3245
1	E	0.35	0/2388	0.53	0/3237
1	F	0.36	0/2395	0.54	0/3246
1	G	0.34	0/2407	0.52	0/3264
1	H	0.35	0/2406	0.51	0/3262
1	I	0.35	0/2409	0.51	0/3266
1	J	0.32	0/2376	0.49	0/3223
1	K	0.33	0/2394	0.50	0/3245
1	L	0.33	0/2390	0.51	0/3240
All	All	0.34	0/28767	0.52	0/39005

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2341	0	2231	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2352	0	2251	11	0
1	C	2345	0	2238	12	0
1	D	2336	0	2229	10	0
1	E	2331	0	2233	12	0
1	F	2338	0	2239	13	0
1	G	2350	0	2247	10	0
1	H	2349	0	2249	18	0
1	I	2352	0	2251	22	0
1	J	2319	0	2211	9	0
1	K	2337	0	2237	9	1
1	L	2333	0	2230	11	0
2	A	57	0	37	16	0
2	B	57	0	37	8	0
2	C	57	0	37	2	0
2	D	57	0	37	4	0
2	E	57	0	37	5	0
2	F	57	0	37	7	0
2	G	57	0	37	3	0
2	H	57	0	37	14	0
2	I	57	0	37	14	0
2	J	57	0	37	5	0
2	K	57	0	37	7	0
2	L	57	0	37	6	0
3	B	10	0	14	0	0
3	D	10	0	14	0	0
3	G	10	0	14	0	0
3	J	10	0	14	2	0
4	A	349	0	0	2	0
4	B	325	0	0	1	1
4	C	326	0	0	1	0
4	D	296	0	0	2	0
4	E	331	0	0	4	0
4	F	347	0	0	2	0
4	G	366	0	0	1	0
4	H	330	0	0	3	0
4	I	344	0	0	3	0
4	J	266	0	0	3	0
4	K	281	0	0	1	0
4	L	295	0	0	1	0
All	All	32663	0	27346	174	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 3.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:2NE:H9	1:G:14:ALA:N	1.24	1.29
1:I:115:TYR:CE2	2:I:401:2NE:C56	2.17	1.28
1:H:115:TYR:CE2	2:H:401:2NE:C56	2.31	1.13
1:I:115:TYR:CE2	2:I:401:2NE:H39	1.83	1.07
1:C:14:ALA:N	2:H:401:2NE:H9	1.52	1.06
2:A:401:2NE:O07	1:G:14:ALA:N	1.88	1.04
1:A:105:GLY:H	2:A:401:2NE:H40	1.20	1.03
1:B:14:ALA:N	2:I:401:2NE:H9	1.57	1.00
2:B:401:2NE:H9	1:I:14:ALA:N	1.62	0.97
1:A:61:PHE:CE1	2:A:401:2NE:H39	2.01	0.95
1:I:115:TYR:HE2	2:I:401:2NE:C56	1.78	0.93
1:A:105:GLY:N	2:A:401:2NE:H40	1.86	0.89
1:A:107:GLN:NE2	2:A:401:2NE:H33	1.90	0.86
1:L:115:TYR:CE2	2:L:401:2NE:C56	2.59	0.85
1:C:14:ALA:N	2:H:401:2NE:O07	2.11	0.84
1:B:14:ALA:N	2:I:401:2NE:O07	2.13	0.82
1:I:115:TYR:CD2	2:I:401:2NE:H39	2.16	0.81
1:H:115:TYR:HE2	2:H:401:2NE:C56	1.94	0.80
1:I:115:TYR:CE2	2:I:401:2NE:C57	2.65	0.80
1:A:61:PHE:CZ	2:A:401:2NE:H39	2.16	0.80
1:H:115:TYR:CE2	2:H:401:2NE:H39	2.14	0.79
1:D:41:ARG:NH1	4:D:783:HOH:O	2.17	0.78
1:I:115:TYR:CZ	2:I:401:2NE:C57	2.66	0.78
1:H:105:GLY:HA3	2:H:401:2NE:H40	1.64	0.78
1:L:105:GLY:HA3	2:L:401:2NE:H40	1.66	0.77
1:F:115:TYR:CE2	2:F:401:2NE:C56	2.68	0.77
1:A:107:GLN:NE2	2:A:401:2NE:C46	2.50	0.74
1:K:103:SER:O	2:K:401:2NE:H30	1.91	0.71
2:K:401:2NE:O08	4:K:741:HOH:O	2.11	0.69
1:F:202:ARG:NH1	4:F:620:HOH:O	2.26	0.68
1:I:105:GLY:HA3	2:I:401:2NE:H40	1.76	0.67
1:I:115:TYR:CZ	2:I:401:2NE:H40	2.30	0.66
1:A:103:SER:O	2:A:401:2NE:H30	1.94	0.66
2:B:401:2NE:O07	1:I:14:ALA:N	2.29	0.65
1:A:61:PHE:HE1	2:A:401:2NE:H39	1.54	0.64
1:B:188:VAL:HG21	2:B:401:2NE:H34	1.79	0.64
1:E:26:ARG:NH1	4:E:695:HOH:O	2.30	0.63
1:H:115:TYR:CE2	2:H:401:2NE:C57	2.80	0.63
1:A:188:VAL:HG21	2:A:401:2NE:H34	1.80	0.62
1:D:202:ARG:NH1	4:D:626:HOH:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:401:2NE:H32	2:E:401:2NE:O50	1.98	0.62
1:E:30:GLY:O	1:E:71:ARG:NH1	2.33	0.62
1:A:188:VAL:CG2	2:A:401:2NE:H34	2.30	0.62
1:H:116:GLN:NE2	4:H:756:HOH:O	2.20	0.61
1:E:202:ARG:NH1	4:E:675:HOH:O	2.33	0.61
1:I:115:TYR:OH	2:I:401:2NE:C57	2.49	0.61
1:C:202:ARG:NH2	4:C:641:HOH:O	2.33	0.61
1:H:26:ARG:HG2	1:H:43:VAL:HG12	1.83	0.61
2:H:401:2NE:H34	2:H:401:2NE:O44	2.00	0.60
1:A:61:PHE:CZ	2:A:401:2NE:C56	2.84	0.60
1:H:115:TYR:CZ	2:H:401:2NE:C57	2.84	0.60
1:I:166:HIS:HE1	4:I:843:HOH:O	1.84	0.60
2:H:401:2NE:O50	2:H:401:2NE:H32	2.00	0.60
2:F:401:2NE:O50	2:F:401:2NE:H32	2.00	0.59
1:I:311:PRO:HG2	1:I:313:TYR:CZ	2.37	0.59
2:I:401:2NE:H32	2:I:401:2NE:O50	2.02	0.59
1:A:56:GLU:OE1	4:A:517:HOH:O	2.16	0.59
2:L:401:2NE:H32	2:L:401:2NE:O50	2.01	0.59
1:A:259:ARG:NH2	4:A:687:HOH:O	2.36	0.59
1:F:105:GLY:HA3	2:F:401:2NE:H40	1.84	0.59
1:E:124:ASP:HA	4:E:804:HOH:O	2.02	0.58
1:E:259:ARG:NH2	4:E:690:HOH:O	2.36	0.58
1:L:202:ARG:NH1	4:L:600:HOH:O	2.36	0.57
1:L:105:GLY:CA	2:L:401:2NE:H40	2.34	0.57
2:D:401:2NE:O50	2:D:401:2NE:H32	2.04	0.56
1:E:115:TYR:CE2	2:E:401:2NE:C56	2.89	0.56
2:K:401:2NE:O50	2:K:401:2NE:H32	2.04	0.56
1:C:160:GLY:HA3	2:C:401:2NE:H35	1.87	0.56
1:L:115:TYR:CE2	2:L:401:2NE:H39	2.41	0.56
1:H:115:TYR:CD2	2:H:401:2NE:H39	2.40	0.55
1:K:107:GLN:NE2	2:K:401:2NE:H33	2.22	0.55
2:K:401:2NE:S48	2:K:401:2NE:O53	2.63	0.55
1:I:202:ARG:NH1	4:I:627:HOH:O	2.39	0.55
2:A:401:2NE:H35	2:A:401:2NE:O44	2.06	0.54
1:B:202:ARG:NH1	4:B:633:HOH:O	2.41	0.54
1:D:260:MET:SD	1:D:281:GLU:HB3	2.48	0.53
1:F:115:TYR:HE2	2:F:401:2NE:C56	2.20	0.53
1:G:311:PRO:HG2	1:G:313:TYR:CZ	2.44	0.53
1:J:188:VAL:HG21	2:J:401:2NE:H34	1.90	0.52
2:B:401:2NE:O50	2:B:401:2NE:H32	2.08	0.52
1:I:116:GLN:NE2	4:I:606:HOH:O	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:260:MET:SD	1:L:281:GLU:HB3	2.50	0.52
1:A:166:HIS:C	1:A:166:HIS:ND1	2.62	0.52
2:D:401:2NE:H15	2:D:401:2NE:O13	2.10	0.51
1:E:115:TYR:CE2	2:E:401:2NE:H39	2.45	0.51
1:C:311:PRO:HG2	1:C:313:TYR:CZ	2.45	0.51
1:C:122:THR:OG1	1:C:124:ASP:OD1	2.22	0.51
1:G:122:THR:OG1	1:G:124:ASP:OD1	2.25	0.50
1:D:185:ASP:OD1	2:D:401:2NE:S48	2.70	0.49
1:E:195:TYR:O	1:E:199:TYR:HB3	2.12	0.49
2:C:401:2NE:H32	2:C:401:2NE:O50	2.12	0.49
1:A:260:MET:SD	1:A:281:GLU:HB3	2.52	0.49
1:L:31:PHE:HE2	1:L:71:ARG:HD2	1.77	0.49
1:A:152:CYS:HB2	1:A:169:CYS:SG	2.53	0.49
1:F:160:GLY:HA3	2:F:401:2NE:H35	1.94	0.49
1:B:188:VAL:CG2	2:B:401:2NE:H34	2.41	0.49
1:H:105:GLY:CA	2:H:401:2NE:H40	2.39	0.49
1:B:122:THR:OG1	1:B:124:ASP:OD1	2.21	0.48
2:J:401:2NE:O50	2:J:401:2NE:H32	2.12	0.48
1:H:115:TYR:HE2	2:H:401:2NE:C55	2.26	0.48
1:F:116:GLN:NE2	4:F:658:HOH:O	2.38	0.48
2:B:401:2NE:H15	2:B:401:2NE:O13	2.14	0.48
1:H:202:ARG:NH2	4:H:635:HOH:O	2.47	0.48
1:G:260:MET:SD	1:G:281:GLU:HB3	2.54	0.47
1:F:115:TYR:CE2	2:F:401:2NE:C57	2.97	0.47
2:J:401:2NE:O13	2:J:401:2NE:H15	2.15	0.47
3:J:402:PGE:O1	4:J:542:HOH:O	2.20	0.47
1:H:259:ARG:NH2	4:H:767:HOH:O	2.47	0.47
1:A:122:THR:OG1	1:A:124:ASP:OD1	2.15	0.47
1:D:30:GLY:O	1:D:71:ARG:NH2	2.46	0.47
1:J:202:ARG:NH1	4:J:592:HOH:O	2.48	0.47
1:J:103:SER:O	2:J:401:2NE:H30	2.15	0.47
1:C:292:ALA:HB1	1:D:110:ARG:HH21	1.80	0.46
1:K:107:GLN:NE2	2:K:401:2NE:C46	2.78	0.46
1:I:292:ALA:HB1	1:J:110:ARG:HH21	1.79	0.46
1:L:195:TYR:O	1:L:199:TYR:HB3	2.14	0.46
1:E:26:ARG:HG2	1:E:43:VAL:HG12	1.98	0.45
1:F:115:TYR:CE2	2:F:401:2NE:H39	2.48	0.45
1:K:122:THR:OG1	1:K:124:ASP:OD1	2.32	0.45
1:A:61:PHE:HZ	2:A:401:2NE:C56	2.26	0.45
1:I:166:HIS:HD2	1:I:172:THR:OG1	1.99	0.45
1:B:157:TRP:CE3	2:B:401:2NE:H2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:TYR:HE2	2:E:401:2NE:C56	2.29	0.45
1:A:15:LEU:N	2:G:401:2NE:H9	2.15	0.45
2:K:401:2NE:O13	2:K:401:2NE:H15	2.17	0.45
1:L:115:TYR:HE2	2:L:401:2NE:C56	2.23	0.45
1:G:195:TYR:O	1:G:199:TYR:HB3	2.17	0.45
1:K:159:ALA:HA	1:K:182:LYS:O	2.17	0.45
1:I:260:MET:SD	1:I:281:GLU:HB3	2.57	0.44
2:I:401:2NE:H15	2:I:401:2NE:O13	2.17	0.44
1:B:107:GLN:NE2	2:B:401:2NE:H33	2.32	0.44
1:G:115:TYR:CE2	2:G:401:2NE:C56	3.00	0.44
1:D:195:TYR:O	1:D:199:TYR:HB3	2.17	0.44
1:H:195:TYR:O	1:H:199:TYR:HB3	2.18	0.44
1:J:256:GLN:O	1:J:260:MET:HG2	2.18	0.44
1:A:195:TYR:O	1:A:199:TYR:HB3	2.17	0.44
1:K:256:GLN:O	1:K:260:MET:HG2	2.17	0.44
1:F:260:MET:SD	1:F:281:GLU:HB3	2.57	0.44
1:C:195:TYR:O	1:C:199:TYR:HB3	2.17	0.44
1:F:195:TYR:O	1:F:199:TYR:HB3	2.17	0.43
1:A:110:ARG:HH11	1:F:292:ALA:HB1	1.83	0.43
1:L:81:ASP:OD1	1:L:81:ASP:N	2.49	0.43
1:K:260:MET:SD	1:K:281:GLU:HB3	2.59	0.43
1:C:260:MET:SD	1:C:281:GLU:HB3	2.59	0.43
1:D:25:TRP:HB3	1:D:40:HIS:HB3	2.01	0.43
1:G:202:ARG:NH1	4:G:661:HOH:O	2.51	0.43
1:J:260:MET:SD	1:J:281:GLU:HB3	2.59	0.43
1:G:159:ALA:HA	1:G:182:LYS:O	2.19	0.42
1:G:115:TYR:CE2	2:G:401:2NE:H39	2.54	0.42
1:H:260:MET:SD	1:H:281:GLU:HB3	2.59	0.42
1:I:157:TRP:CE3	2:I:401:2NE:H2	2.54	0.42
1:D:103:SER:O	2:D:401:2NE:H30	2.19	0.42
1:J:195:TYR:O	1:J:199:TYR:HB3	2.20	0.42
1:B:195:TYR:O	1:B:199:TYR:HB3	2.20	0.42
1:K:81:ASP:OD1	1:K:81:ASP:N	2.50	0.42
1:A:107:GLN:NE2	2:A:401:2NE:H32	2.30	0.42
1:B:275:GLN:OE1	1:F:268:LEU:HG	2.20	0.42
1:H:113:SER:HB2	1:I:313:TYR:CE1	2.56	0.41
3:J:402:PGE:H2	1:L:202:ARG:HA	2.02	0.41
1:A:159:ALA:HA	1:A:182:LYS:O	2.21	0.41
1:K:195:TYR:O	1:K:199:TYR:HB3	2.21	0.41
1:H:115:TYR:OH	2:H:401:2NE:C57	2.68	0.41
1:I:195:TYR:O	1:I:199:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:401:2NE:O08	4:J:720:HOH:O	2.22	0.41
2:E:401:2NE:O13	2:E:401:2NE:H15	2.21	0.41
1:F:51:ALA:HA	1:F:88:THR:O	2.21	0.40
1:H:159:ALA:HA	1:H:182:LYS:O	2.21	0.40
1:B:260:MET:SD	1:B:281:GLU:HB3	2.61	0.40
1:C:268:LEU:HG	1:E:275:GLN:OE1	2.22	0.40
1:C:287:TYR:HD2	1:D:114:GLY:HA2	1.87	0.40
1:E:310:PHE:HA	1:E:311:PRO:HD2	1.93	0.40
1:C:256:GLN:O	1:C:260:MET:HG2	2.21	0.40
1:I:292:ALA:HB1	1:J:110:ARG:NH2	2.36	0.40
1:J:51:ALA:HA	1:J:88:THR:O	2.22	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:K:124:ASP:OD2	4:B:792:HOH:O[2_1048]	2.15	0.05

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	298/334 (89%)	291 (98%)	7 (2%)	0	100	100
1	B	299/334 (90%)	293 (98%)	6 (2%)	0	100	100
1	C	299/334 (90%)	292 (98%)	7 (2%)	0	100	100
1	D	297/334 (89%)	291 (98%)	6 (2%)	0	100	100
1	E	296/334 (89%)	291 (98%)	5 (2%)	0	100	100
1	F	296/334 (89%)	290 (98%)	6 (2%)	0	100	100
1	G	299/334 (90%)	294 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	299/334 (90%)	293 (98%)	6 (2%)	0	100	100
1	I	299/334 (90%)	294 (98%)	5 (2%)	0	100	100
1	J	295/334 (88%)	289 (98%)	6 (2%)	0	100	100
1	K	296/334 (89%)	290 (98%)	6 (2%)	0	100	100
1	L	296/334 (89%)	289 (98%)	7 (2%)	0	100	100
All	All	3569/4008 (89%)	3497 (98%)	72 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	235/264 (89%)	233 (99%)	2 (1%)	78	63
1	B	236/264 (89%)	235 (100%)	1 (0%)	91	84
1	C	234/264 (89%)	233 (100%)	1 (0%)	91	84
1	D	234/264 (89%)	233 (100%)	1 (0%)	91	84
1	E	233/264 (88%)	232 (100%)	1 (0%)	91	84
1	F	235/264 (89%)	234 (100%)	1 (0%)	91	84
1	G	236/264 (89%)	234 (99%)	2 (1%)	81	68
1	H	235/264 (89%)	234 (100%)	1 (0%)	91	84
1	I	236/264 (89%)	235 (100%)	1 (0%)	91	84
1	J	232/264 (88%)	231 (100%)	1 (0%)	91	84
1	K	235/264 (89%)	233 (99%)	2 (1%)	78	63
1	L	234/264 (89%)	233 (100%)	1 (0%)	91	84
All	All	2815/3168 (89%)	2800 (100%)	15 (0%)	88	80

All (15) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	165	LEU
1	A	166	HIS
1	B	166	HIS
1	C	166	HIS
1	D	166	HIS
1	E	166	HIS
1	F	166	HIS
1	G	32	ASP
1	G	166	HIS
1	H	166	HIS
1	I	166	HIS
1	J	166	HIS
1	K	124	ASP
1	K	166	HIS
1	L	166	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	166	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 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	$\# Z  > 2$
3	PGE	J	402	-	9,9,9	0.31	0	8,8,8	0.66	0
3	PGE	D	402	-	9,9,9	0.26	0	8,8,8	0.46	0
3	PGE	B	402	-	9,9,9	0.28	0	8,8,8	0.33	0
3	PGE	G	402	-	9,9,9	0.27	0	8,8,8	0.63	0
2	2NE	B	401	-	52,60,60	2.70	8 (15%)	66,89,89	2.25	13 (19%)
2	2NE	C	401	-	52,60,60	2.79	10 (19%)	66,89,89	2.11	10 (15%)
2	2NE	F	401	-	52,60,60	2.73	9 (17%)	66,89,89	2.22	11 (16%)
2	2NE	A	401	-	52,60,60	2.79	10 (19%)	66,89,89	2.04	11 (16%)
2	2NE	D	401	-	52,60,60	2.81	9 (17%)	66,89,89	2.30	10 (15%)
2	2NE	G	401	-	52,60,60	2.70	9 (17%)	66,89,89	2.20	9 (13%)
2	2NE	J	401	-	52,60,60	2.84	10 (19%)	66,89,89	2.27	11 (16%)
2	2NE	E	401	-	52,60,60	2.80	8 (15%)	66,89,89	2.24	11 (16%)
2	2NE	H	401	-	52,60,60	2.72	10 (19%)	66,89,89	2.12	9 (13%)
2	2NE	K	401	-	52,60,60	2.78	11 (21%)	66,89,89	2.16	10 (15%)
2	2NE	I	401	-	52,60,60	2.81	10 (19%)	66,89,89	2.21	12 (18%)
2	2NE	L	401	-	52,60,60	2.76	10 (19%)	66,89,89	2.26	14 (21%)

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
3	PGE	J	402	-	-	5/7/7/7	-
3	PGE	D	402	-	-	2/7/7/7	-
3	PGE	B	402	-	-	2/7/7/7	-
3	PGE	G	402	-	-	4/7/7/7	-
2	2NE	B	401	-	-	8/51/71/71	0/4/4/4
2	2NE	C	401	-	-	5/51/71/71	0/4/4/4
2	2NE	F	401	-	-	5/51/71/71	0/4/4/4
2	2NE	A	401	-	-	11/51/71/71	0/4/4/4
2	2NE	D	401	-	-	9/51/71/71	0/4/4/4
2	2NE	G	401	-	-	6/51/71/71	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2NE	J	401	-	-	11/51/71/71	0/4/4/4
2	2NE	E	401	-	-	2/51/71/71	0/4/4/4
2	2NE	H	401	-	-	3/51/71/71	0/4/4/4
2	2NE	K	401	-	-	6/51/71/71	0/4/4/4
2	2NE	I	401	-	-	4/51/71/71	0/4/4/4
2	2NE	L	401	-	-	7/51/71/71	0/4/4/4

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	401	2NE	C18-C17	-15.30	1.30	1.53
2	E	401	2NE	C18-C17	-15.14	1.30	1.53
2	D	401	2NE	C18-C17	-15.07	1.30	1.53
2	I	401	2NE	C18-C17	-14.89	1.31	1.53
2	L	401	2NE	C18-C17	-14.71	1.31	1.53
2	C	401	2NE	C18-C17	-14.59	1.31	1.53
2	A	401	2NE	C18-C17	-14.48	1.31	1.53
2	F	401	2NE	C18-C17	-14.46	1.31	1.53
2	K	401	2NE	C18-C17	-14.28	1.32	1.53
2	B	401	2NE	C18-C17	-14.28	1.32	1.53
2	G	401	2NE	C18-C17	-13.86	1.32	1.53
2	H	401	2NE	C18-C17	-13.71	1.33	1.53
2	D	401	2NE	O16-C15	-7.94	1.27	1.45
2	J	401	2NE	O16-C15	-7.91	1.27	1.45
2	H	401	2NE	O16-C15	-7.88	1.27	1.45
2	C	401	2NE	O16-C15	-7.79	1.27	1.45
2	G	401	2NE	O16-C15	-7.75	1.27	1.45
2	I	401	2NE	O16-C15	-7.71	1.27	1.45
2	L	401	2NE	O16-C15	-7.63	1.27	1.45
2	E	401	2NE	O16-C15	-7.59	1.28	1.45
2	K	401	2NE	O16-C15	-7.45	1.28	1.45
2	A	401	2NE	O16-C15	-7.30	1.28	1.45
2	F	401	2NE	O16-C15	-7.27	1.28	1.45
2	B	401	2NE	O16-C15	-7.11	1.29	1.45
2	A	401	2NE	C38-N40	6.18	1.47	1.33
2	F	401	2NE	C38-N40	6.09	1.46	1.33
2	H	401	2NE	C38-N40	6.02	1.46	1.33
2	K	401	2NE	C38-N40	5.96	1.46	1.33
2	G	401	2NE	C38-N40	5.78	1.46	1.33
2	D	401	2NE	C38-N40	5.72	1.46	1.33
2	C	401	2NE	C38-N40	5.64	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	401	2NE	C38-N40	5.56	1.45	1.33
2	B	401	2NE	C38-N40	5.42	1.45	1.33
2	J	401	2NE	C38-N40	5.36	1.45	1.33
2	A	401	2NE	C43-N45	5.20	1.45	1.33
2	E	401	2NE	C38-N40	5.18	1.44	1.33
2	L	401	2NE	C38-N40	5.01	1.44	1.33
2	D	401	2NE	C43-N45	4.90	1.44	1.33
2	I	401	2NE	C43-N45	4.90	1.44	1.33
2	B	401	2NE	C43-N45	4.87	1.44	1.33
2	K	401	2NE	C43-N45	4.86	1.44	1.33
2	G	401	2NE	C43-N45	4.84	1.44	1.33
2	C	401	2NE	C43-N45	4.84	1.44	1.33
2	H	401	2NE	C43-N45	4.81	1.44	1.33
2	L	401	2NE	C43-N45	4.69	1.44	1.33
2	F	401	2NE	C43-N45	4.65	1.44	1.33
2	J	401	2NE	C43-N45	4.63	1.43	1.33
2	E	401	2NE	C43-N45	4.51	1.43	1.33
2	J	401	2NE	O19-C18	3.99	1.52	1.43
2	K	401	2NE	O19-C18	3.96	1.52	1.43
2	I	401	2NE	O19-C18	3.96	1.52	1.43
2	F	401	2NE	O19-C18	3.96	1.52	1.43
2	B	401	2NE	O19-C18	3.96	1.52	1.43
2	A	401	2NE	O19-C18	3.96	1.52	1.43
2	L	401	2NE	O19-C18	3.96	1.52	1.43
2	E	401	2NE	O19-C18	3.95	1.52	1.43
2	G	401	2NE	O19-C18	3.94	1.52	1.43
2	H	401	2NE	O19-C18	3.94	1.52	1.43
2	D	401	2NE	O19-C18	3.93	1.52	1.43
2	C	401	2NE	O19-C18	3.92	1.52	1.43
2	K	401	2NE	C33-N34	3.02	1.37	1.32
2	E	401	2NE	C33-N34	2.80	1.36	1.32
2	C	401	2NE	C33-N34	2.72	1.36	1.32
2	F	401	2NE	C33-N34	2.71	1.36	1.32
2	F	401	2NE	C30-N31	2.67	1.43	1.34
2	H	401	2NE	C30-N31	2.67	1.43	1.34
2	D	401	2NE	C30-N31	2.67	1.43	1.34
2	L	401	2NE	C30-N31	2.67	1.43	1.34
2	A	401	2NE	C30-N31	2.67	1.43	1.34
2	J	401	2NE	C30-N31	2.66	1.43	1.34
2	E	401	2NE	C30-N31	2.66	1.43	1.34
2	I	401	2NE	C30-N31	2.66	1.43	1.34
2	G	401	2NE	C30-N31	2.66	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	2NE	C30-N31	2.66	1.43	1.34
2	C	401	2NE	C30-N31	2.65	1.43	1.34
2	K	401	2NE	C30-N31	2.65	1.43	1.34
2	H	401	2NE	C29-C35	-2.57	1.34	1.40
2	A	401	2NE	C42-C43	2.48	1.56	1.51
2	A	401	2NE	C33-N34	2.46	1.36	1.32
2	L	401	2NE	C33-N34	2.46	1.36	1.32
2	B	401	2NE	C33-N34	2.37	1.35	1.32
2	D	401	2NE	C33-N34	2.37	1.35	1.32
2	H	401	2NE	C33-N34	2.31	1.35	1.32
2	K	401	2NE	C29-C35	-2.29	1.34	1.40
2	I	401	2NE	C33-N34	2.18	1.35	1.32
2	G	401	2NE	C29-C35	-2.13	1.35	1.40
2	H	401	2NE	O53-C52	2.12	1.40	1.36
2	F	401	2NE	O53-C52	2.12	1.40	1.36
2	I	401	2NE	O37-C36	-2.11	1.38	1.42
2	L	401	2NE	O53-C52	2.10	1.40	1.36
2	D	401	2NE	O53-C52	2.10	1.40	1.36
2	J	401	2NE	O53-C52	2.10	1.40	1.36
2	C	401	2NE	O53-C52	2.10	1.40	1.36
2	C	401	2NE	O21-C20	-2.09	1.36	1.44
2	I	401	2NE	O53-C52	2.09	1.40	1.36
2	K	401	2NE	O53-C52	2.08	1.40	1.36
2	A	401	2NE	O53-C52	2.08	1.40	1.36
2	B	401	2NE	O53-C52	2.08	1.40	1.36
2	E	401	2NE	O53-C52	2.07	1.40	1.36
2	A	401	2NE	O37-C36	-2.07	1.38	1.42
2	G	401	2NE	O53-C52	2.07	1.40	1.36
2	J	401	2NE	O37-C36	-2.05	1.38	1.42
2	I	401	2NE	C33-N32	2.05	1.37	1.33
2	K	401	2NE	C42-C43	2.04	1.55	1.51
2	L	401	2NE	O37-C36	-2.04	1.38	1.42
2	L	401	2NE	C29-C35	-2.04	1.35	1.40
2	F	401	2NE	O37-C36	-2.04	1.38	1.42
2	H	401	2NE	O37-C36	-2.03	1.38	1.42
2	D	401	2NE	O37-C36	-2.02	1.38	1.42
2	G	401	2NE	O37-C36	-2.02	1.38	1.42
2	J	401	2NE	O21-C20	-2.02	1.36	1.44
2	K	401	2NE	C33-N32	2.01	1.37	1.33
2	C	401	2NE	O37-C36	-2.01	1.38	1.42
2	J	401	2NE	C33-N34	2.00	1.35	1.32

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	2NE	C29-C30-N31	11.72	138.16	120.35
2	A	401	2NE	C29-C30-N31	11.61	138.00	120.35
2	G	401	2NE	C29-C30-N31	11.51	137.84	120.35
2	J	401	2NE	C29-C30-N31	11.42	137.70	120.35
2	B	401	2NE	C29-C30-N31	11.37	137.62	120.35
2	H	401	2NE	C29-C30-N31	11.35	137.60	120.35
2	I	401	2NE	C29-C30-N31	11.35	137.60	120.35
2	L	401	2NE	C29-C30-N31	11.25	137.46	120.35
2	E	401	2NE	C29-C30-N31	11.17	137.33	120.35
2	C	401	2NE	C29-C30-N31	11.07	137.17	120.35
2	K	401	2NE	C29-C30-N31	11.06	137.17	120.35
2	F	401	2NE	C29-C30-N31	11.06	137.16	120.35
2	F	401	2NE	N31-C30-N32	-7.53	102.94	118.57
2	K	401	2NE	N31-C30-N32	-7.52	102.97	118.57
2	C	401	2NE	N31-C30-N32	-7.51	102.99	118.57
2	E	401	2NE	N31-C30-N32	-7.45	103.11	118.57
2	L	401	2NE	N31-C30-N32	-7.37	103.27	118.57
2	B	401	2NE	C41-C42-C43	-7.33	100.14	112.36
2	I	401	2NE	N31-C30-N32	-7.32	103.37	118.57
2	H	401	2NE	N31-C30-N32	-7.29	103.44	118.57
2	B	401	2NE	N31-C30-N32	-7.29	103.44	118.57
2	D	401	2NE	C41-C42-C43	-7.29	100.22	112.36
2	G	401	2NE	C41-C42-C43	-7.29	100.22	112.36
2	J	401	2NE	N31-C30-N32	-7.26	103.50	118.57
2	G	401	2NE	N31-C30-N32	-7.20	103.63	118.57
2	A	401	2NE	N31-C30-N32	-7.10	103.83	118.57
2	D	401	2NE	N31-C30-N32	-7.05	103.95	118.57
2	F	401	2NE	C41-C42-C43	-6.95	100.79	112.36
2	E	401	2NE	C41-C42-C43	-6.39	101.72	112.36
2	J	401	2NE	C41-C42-C43	-6.38	101.74	112.36
2	L	401	2NE	C41-C42-C43	-6.18	102.06	112.36
2	D	401	2NE	C18-C20-C15	-5.33	93.77	103.22
2	K	401	2NE	N34-C33-N32	-5.17	120.60	128.68
2	C	401	2NE	C41-C42-C43	-4.80	104.37	112.36
2	I	401	2NE	C41-C42-C43	-4.62	104.66	112.36
2	F	401	2NE	C18-C20-C15	-4.53	95.20	103.22
2	L	401	2NE	C41-N40-C38	-4.41	114.73	122.59
2	I	401	2NE	C18-C20-C15	-4.40	95.42	103.22
2	K	401	2NE	C18-C20-C15	-4.24	95.71	103.22
2	E	401	2NE	C18-C20-C15	-4.19	95.80	103.22
2	K	401	2NE	C41-C42-C43	-4.17	105.42	112.36
2	C	401	2NE	C18-C20-C15	-4.15	95.88	103.22
2	J	401	2NE	C41-N40-C38	-4.11	115.25	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	2NE	C18-C20-C15	-4.05	96.05	103.22
2	H	401	2NE	C41-C42-C43	-3.95	105.79	112.36
2	B	401	2NE	C18-C20-C15	-3.85	96.39	103.22
2	I	401	2NE	O05-C04-C02	-3.85	104.36	110.55
2	L	401	2NE	C18-C20-C15	-3.77	96.53	103.22
2	A	401	2NE	C18-C20-C15	-3.76	96.56	103.22
2	G	401	2NE	C18-C20-C15	-3.75	96.58	103.22
2	J	401	2NE	C18-C20-C15	-3.73	96.61	103.22
2	H	401	2NE	N34-C33-N32	-3.69	122.92	128.68
2	E	401	2NE	N34-C33-N32	-3.68	122.93	128.68
2	C	401	2NE	N34-C33-N32	-3.64	122.99	128.68
2	E	401	2NE	C46-N45-C43	-3.62	116.11	122.84
2	B	401	2NE	N34-C33-N32	-3.57	123.10	128.68
2	I	401	2NE	N34-C33-N32	-3.55	123.13	128.68
2	E	401	2NE	C41-N40-C38	-3.47	116.41	122.59
2	J	401	2NE	C42-C43-N45	3.46	122.25	116.42
2	J	401	2NE	C46-N45-C43	-3.36	116.61	122.84
2	L	401	2NE	N34-C33-N32	-3.32	123.49	128.68
2	A	401	2NE	N34-C33-N32	-3.30	123.53	128.68
2	F	401	2NE	N34-C33-N32	-3.28	123.55	128.68
2	H	401	2NE	O05-C04-C02	-3.26	105.31	110.55
2	L	401	2NE	O50-C49-C51	-3.26	118.40	123.25
2	I	401	2NE	C51-C49-S48	3.23	121.19	114.94
2	D	401	2NE	P10-O09-P06	-3.20	121.85	132.83
2	I	401	2NE	C41-N40-C38	-3.15	116.98	122.59
2	D	401	2NE	C41-N40-C38	-3.12	117.03	122.59
2	L	401	2NE	C51-C49-S48	3.04	120.82	114.94
2	J	401	2NE	P10-O09-P06	-2.97	122.63	132.83
2	G	401	2NE	O05-C04-C02	-2.95	105.81	110.55
2	L	401	2NE	O05-C04-C02	-2.94	105.82	110.55
2	K	401	2NE	C42-C41-N40	2.93	117.80	111.90
2	H	401	2NE	O50-C49-C51	-2.91	118.91	123.25
2	B	401	2NE	C41-N40-C38	-2.84	117.52	122.59
2	J	401	2NE	O50-C49-C51	-2.79	119.10	123.25
2	B	401	2NE	O05-C04-C02	-2.76	106.11	110.55
2	C	401	2NE	O05-C04-C02	-2.73	106.15	110.55
2	E	401	2NE	O50-C49-C51	-2.70	119.23	123.25
2	F	401	2NE	C46-N45-C43	-2.70	117.83	122.84
2	I	401	2NE	C42-C41-N40	2.69	117.32	111.90
2	K	401	2NE	C20-C18-C17	2.68	105.84	99.89
2	I	401	2NE	O50-C49-C51	-2.67	119.27	123.25
2	G	401	2NE	C47-C46-N45	-2.66	106.83	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	2NE	C42-C41-N40	2.66	117.26	111.90
2	G	401	2NE	N34-C33-N32	-2.66	124.52	128.68
2	E	401	2NE	O44-C43-C42	-2.62	117.23	122.02
2	C	401	2NE	C51-C49-S48	2.61	120.00	114.94
2	H	401	2NE	C51-C49-S48	2.61	119.99	114.94
2	H	401	2NE	C47-S48-C49	-2.60	96.53	99.80
2	K	401	2NE	P10-O09-P06	-2.57	124.02	132.83
2	J	401	2NE	O44-C43-C42	-2.56	117.34	122.02
2	A	401	2NE	O44-C43-C42	-2.49	117.46	122.02
2	K	401	2NE	C47-C46-N45	-2.45	107.28	112.42
2	A	401	2NE	C41-N40-C38	-2.44	118.23	122.59
2	L	401	2NE	C46-N45-C43	-2.39	118.40	122.84
2	D	401	2NE	C35-C29-N28	-2.36	106.94	109.40
2	B	401	2NE	C20-C18-C17	2.36	105.12	99.89
2	F	401	2NE	C20-C18-C17	2.35	105.10	99.89
2	A	401	2NE	C20-C18-C17	2.35	105.09	99.89
2	G	401	2NE	C46-N45-C43	-2.32	118.53	122.84
2	L	401	2NE	C42-C43-N45	2.30	120.29	116.42
2	E	401	2NE	C42-C41-N40	2.26	116.46	111.90
2	C	401	2NE	O13-C14-C15	-2.23	101.30	108.99
2	F	401	2NE	O50-C49-C51	-2.21	119.95	123.25
2	A	401	2NE	C41-C42-C43	-2.21	108.68	112.36
2	L	401	2NE	C42-C41-N40	2.20	116.34	111.90
2	A	401	2NE	C51-C49-S48	2.19	119.19	114.94
2	I	401	2NE	C42-C43-N45	2.18	120.09	116.42
2	C	401	2NE	O50-C49-C51	-2.17	120.01	123.25
2	D	401	2NE	N34-C33-N32	-2.17	125.28	128.68
2	F	401	2NE	C42-C43-N45	2.17	120.08	116.42
2	C	401	2NE	C42-C43-N45	2.16	120.06	116.42
2	G	401	2NE	C41-N40-C38	-2.16	118.74	122.59
2	F	401	2NE	C47-C46-N45	-2.15	107.90	112.42
2	B	401	2NE	C51-C49-S48	2.14	119.08	114.94
2	D	401	2NE	C47-C46-N45	-2.12	107.95	112.42
2	A	401	2NE	P10-O09-P06	-2.11	125.58	132.83
2	F	401	2NE	O05-C04-C02	-2.11	107.16	110.55
2	B	401	2NE	C42-C43-N45	2.08	119.93	116.42
2	B	401	2NE	P10-O09-P06	-2.08	125.69	132.83
2	K	401	2NE	C46-N45-C43	-2.06	119.02	122.84
2	E	401	2NE	P10-O09-P06	-2.05	125.78	132.83
2	D	401	2NE	O05-C04-C02	-2.05	107.25	110.55
2	L	401	2NE	O44-C43-N45	-2.04	119.16	123.01
2	L	401	2NE	C20-C18-C17	2.04	104.41	99.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	2NE	O50-C49-C51	-2.03	120.23	123.25
2	J	401	2NE	C20-C18-C17	2.03	104.38	99.89
2	I	401	2NE	C20-C18-C17	2.01	104.34	99.89
2	B	401	2NE	C46-N45-C43	-2.00	119.12	122.84

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	2NE	P10-O09-P06-O05
2	B	401	2NE	C47-C46-N45-C43
2	B	401	2NE	N45-C46-C47-S48
2	C	401	2NE	S48-C49-C51-C52
2	C	401	2NE	S48-C49-C51-C57
2	F	401	2NE	S48-C49-C51-C57
2	A	401	2NE	C20-O21-P22-O24
2	A	401	2NE	C47-C46-N45-C43
2	A	401	2NE	N45-C46-C47-S48
2	A	401	2NE	O50-C49-S48-C47
2	A	401	2NE	C51-C49-S48-C47
2	D	401	2NE	C04-O05-P06-O08
2	D	401	2NE	C47-C46-N45-C43
2	D	401	2NE	O50-C49-C51-C52
2	G	401	2NE	S48-C49-C51-C52
2	G	401	2NE	O50-C49-C51-C52
2	G	401	2NE	O50-C49-C51-C57
2	J	401	2NE	C04-O05-P06-O08
2	J	401	2NE	N45-C46-C47-S48
2	H	401	2NE	C47-C46-N45-C43
2	K	401	2NE	C47-C46-N45-C43
2	I	401	2NE	S48-C49-C51-C52
2	I	401	2NE	O50-C49-C51-C52
2	I	401	2NE	O50-C49-C51-C57
2	L	401	2NE	O50-C49-C51-C52
2	E	401	2NE	O50-C49-C51-C57
2	H	401	2NE	O50-C49-C51-C57
3	B	402	PGE	O2-C3-C4-O3
3	J	402	PGE	O1-C1-C2-O2
3	G	402	PGE	O2-C3-C4-O3
2	L	401	2NE	O50-C49-C51-C57
2	J	401	2NE	O50-C49-C51-C57
2	D	401	2NE	N45-C46-C47-S48

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Mol	Chain	Res	Type	Atoms
2	K	401	2NE	N45-C46-C47-S48
2	G	401	2NE	C47-C46-N45-C43
2	H	401	2NE	C42-C41-N40-C38
2	B	401	2NE	O50-C49-C51-C57
3	J	402	PGE	O2-C3-C4-O3
2	A	401	2NE	O50-C49-C51-C57
2	C	401	2NE	O50-C49-C51-C57
2	F	401	2NE	O50-C49-C51-C57
2	F	401	2NE	P10-O09-P06-O05
2	A	401	2NE	P10-O09-P06-O05
2	L	401	2NE	P10-O09-P06-O05
3	G	402	PGE	C1-C2-O2-C3
3	D	402	PGE	C4-C3-O2-C2
3	G	402	PGE	C3-C4-O3-C5
2	B	401	2NE	C20-O21-P22-O25
2	J	401	2NE	C20-O21-P22-O24
2	J	401	2NE	C20-O21-P22-O25
2	B	401	2NE	S48-C49-C51-C52
2	B	401	2NE	S48-C49-C51-C57
2	F	401	2NE	S48-C49-C51-C52
2	A	401	2NE	S48-C49-C51-C52
2	A	401	2NE	S48-C49-C51-C57
2	D	401	2NE	S48-C49-C51-C52
2	D	401	2NE	S48-C49-C51-C57
2	J	401	2NE	S48-C49-C51-C52
2	J	401	2NE	S48-C49-C51-C57
2	K	401	2NE	S48-C49-C51-C52
2	K	401	2NE	S48-C49-C51-C57
2	L	401	2NE	S48-C49-C51-C52
2	L	401	2NE	S48-C49-C51-C57
2	B	401	2NE	O50-C49-C51-C52
2	C	401	2NE	O50-C49-C51-C52
2	F	401	2NE	O50-C49-C51-C52
2	A	401	2NE	O50-C49-C51-C52
2	J	401	2NE	O50-C49-C51-C52
2	K	401	2NE	O50-C49-C51-C52
2	D	401	2NE	O50-C49-C51-C57
2	J	401	2NE	P10-O09-P06-O08
3	J	402	PGE	O3-C5-C6-O4
3	J	402	PGE	C4-C3-O2-C2
2	L	401	2NE	C42-C41-N40-C38
2	E	401	2NE	C47-C46-N45-C43

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Mol	Chain	Res	Type	Atoms
2	L	401	2NE	C47-C46-N45-C43
3	B	402	PGE	C4-C3-O2-C2
2	D	401	2NE	C20-O21-P 22-O23
2	A	401	2NE	C01-C02-C04-O05
2	G	401	2NE	N45-C46-C47-S48
2	J	401	2NE	C47-C46-N45-C43
3	J	402	PGE	C1-C2-O2-C3
2	C	401	2NE	C20-O21-P 22-O24
2	D	401	2NE	C20-O21-P 22-O25
2	J	401	2NE	C04-O05-P06-O09
3	D	402	PGE	O2-C3-C4-O3
2	K	401	2NE	C04-O05-P06-O08
2	G	401	2NE	S48-C49-C51-C57
2	I	401	2NE	S48-C49-C51-C57
3	G	402	PGE	C6-C5-O3-C4

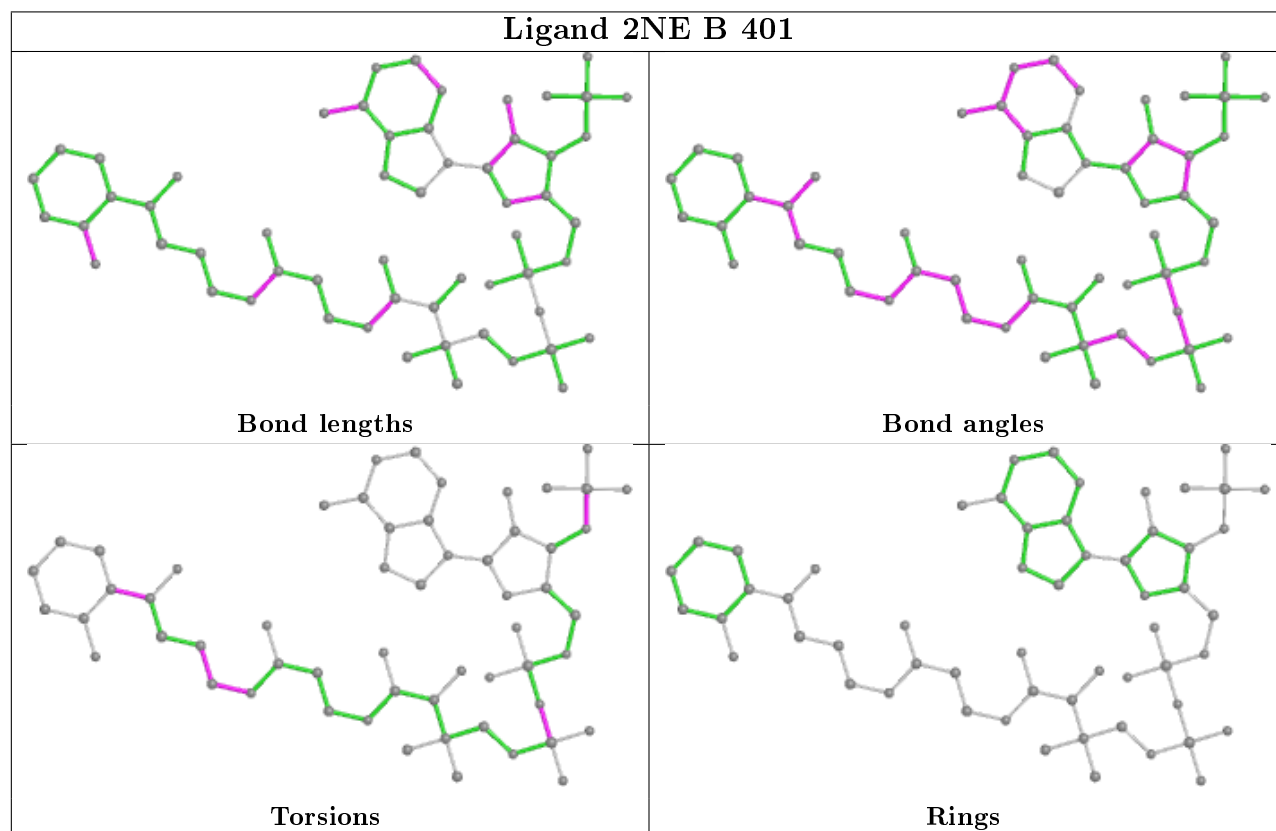
There are no ring outliers.

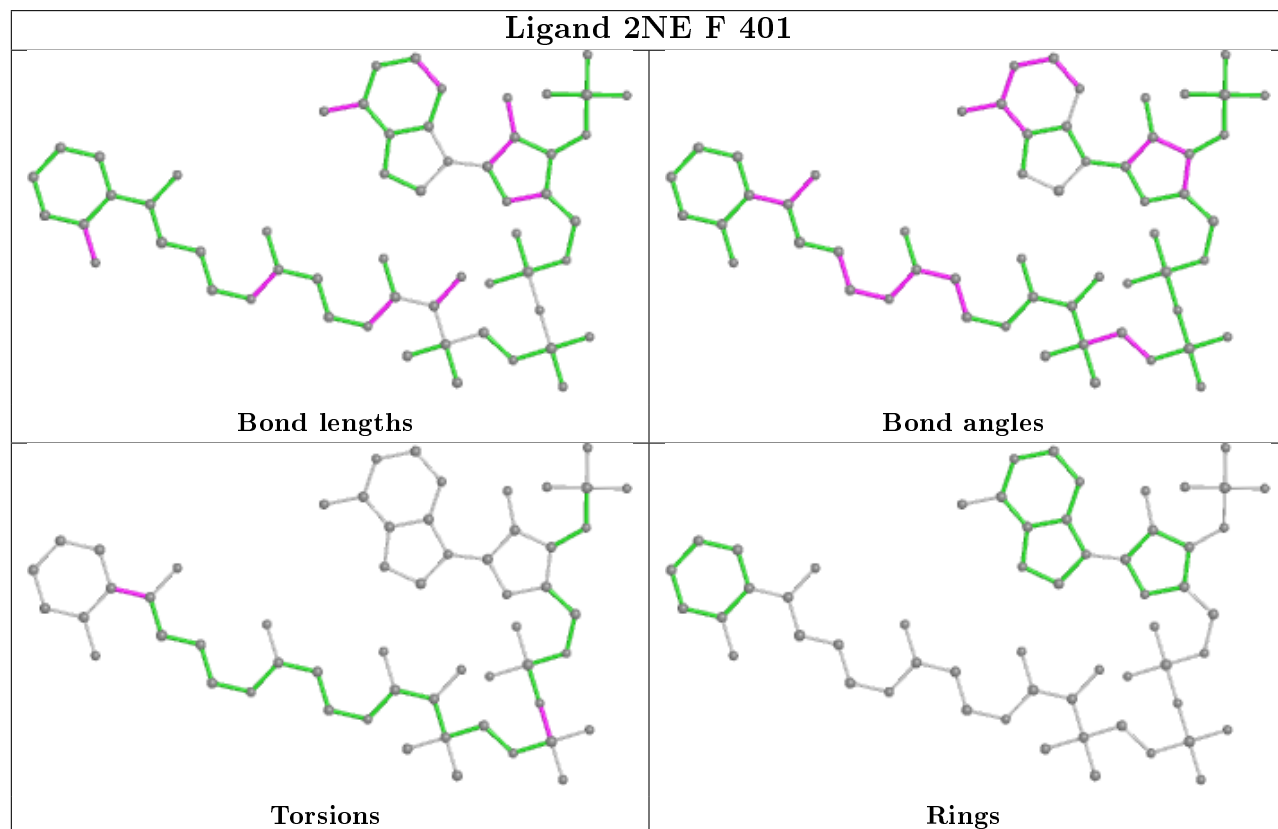
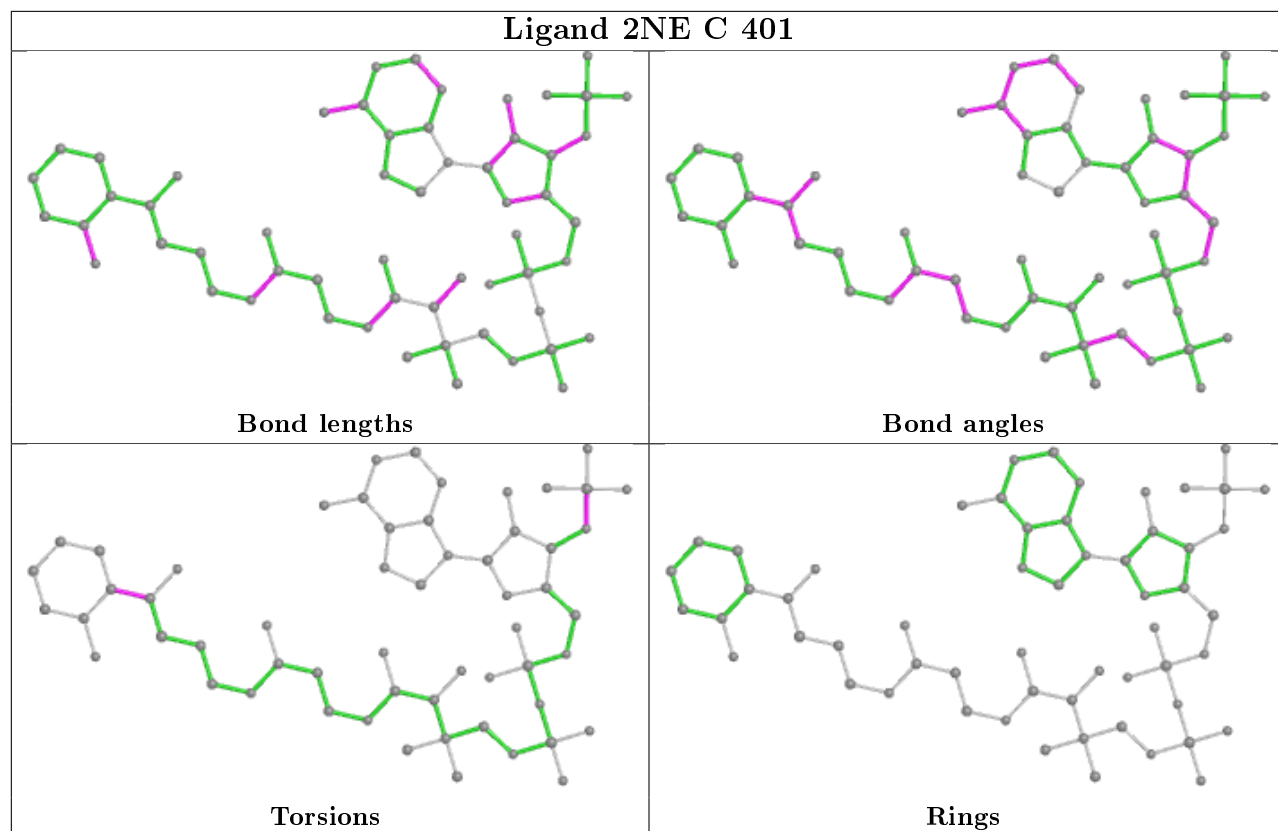
13 monomers are involved in 93 short contacts:

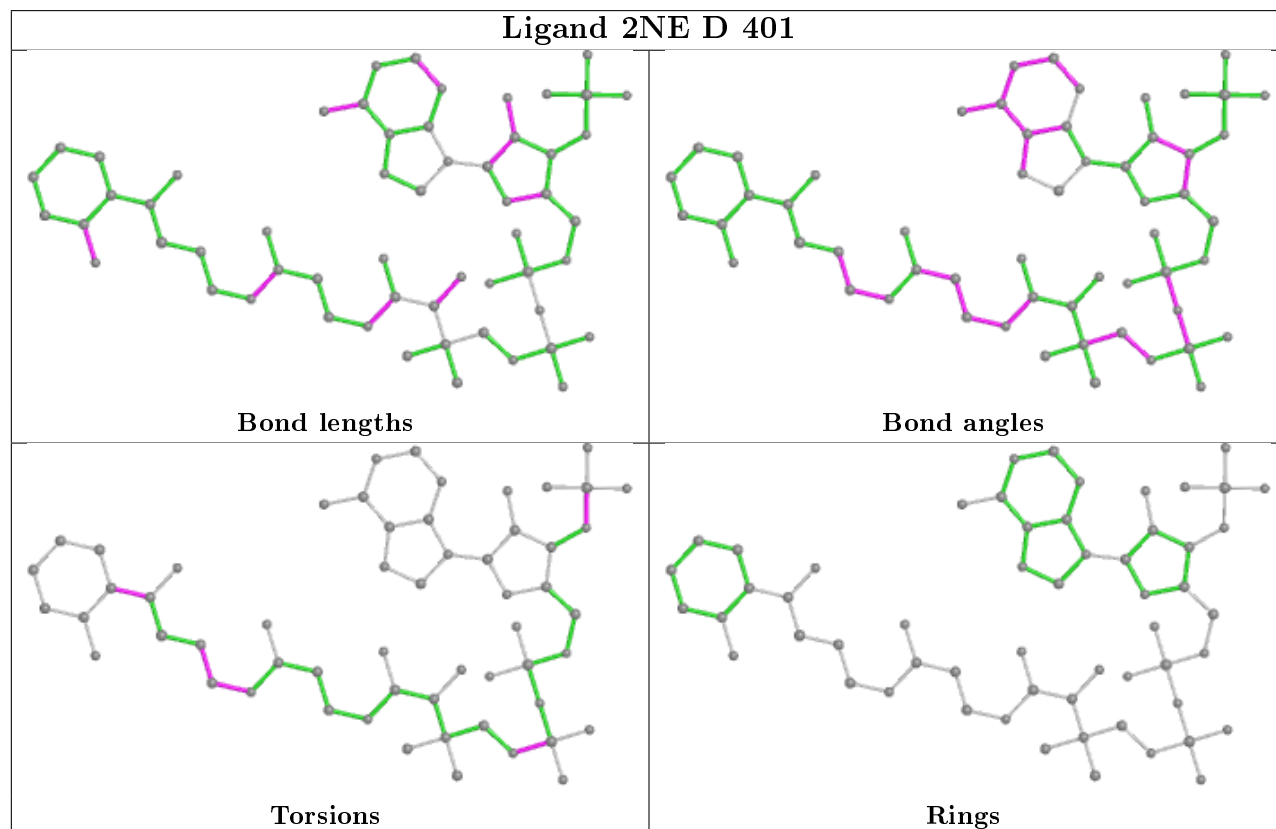
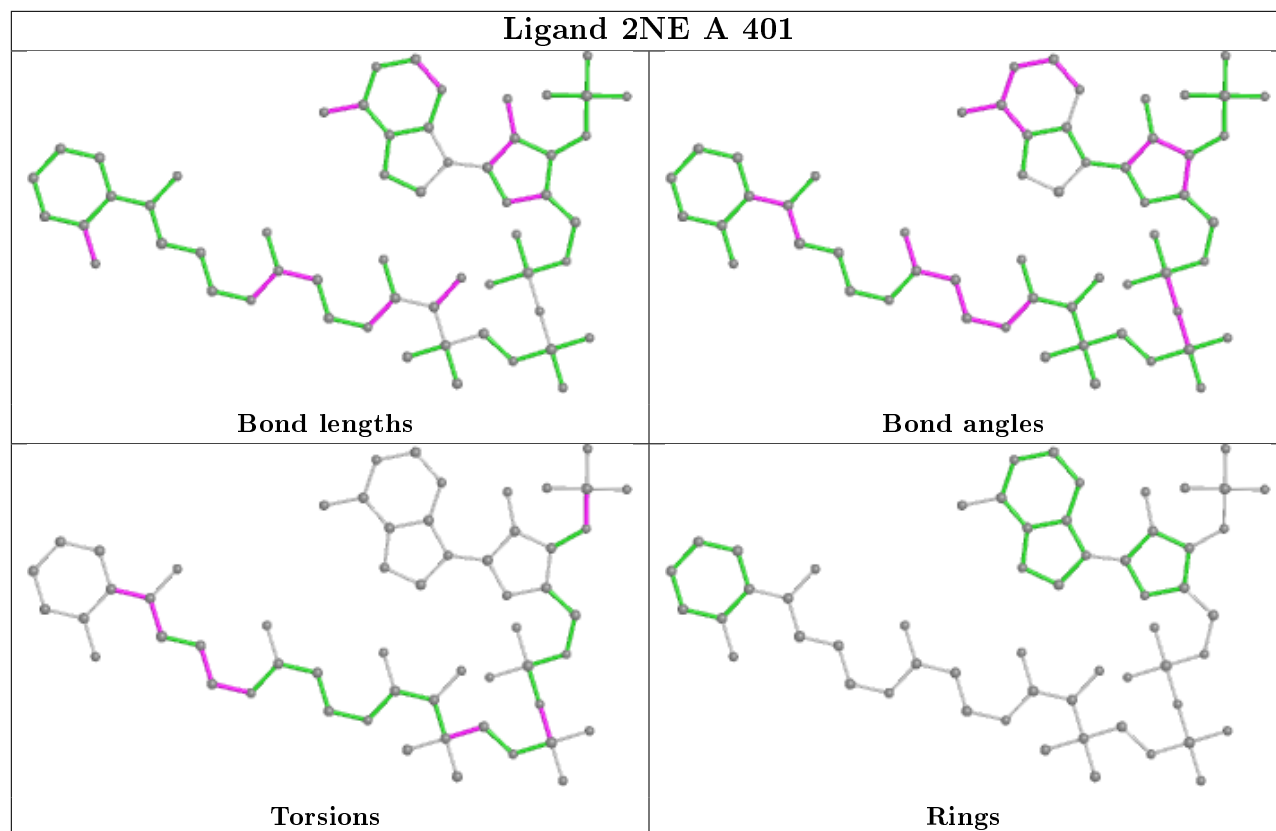
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	402	PGE	2	0
2	B	401	2NE	8	0
2	C	401	2NE	2	0
2	F	401	2NE	7	0
2	A	401	2NE	16	0
2	D	401	2NE	4	0
2	G	401	2NE	3	0
2	J	401	2NE	5	0
2	E	401	2NE	5	0
2	H	401	2NE	14	0
2	K	401	2NE	7	0
2	I	401	2NE	14	0
2	L	401	2NE	6	0

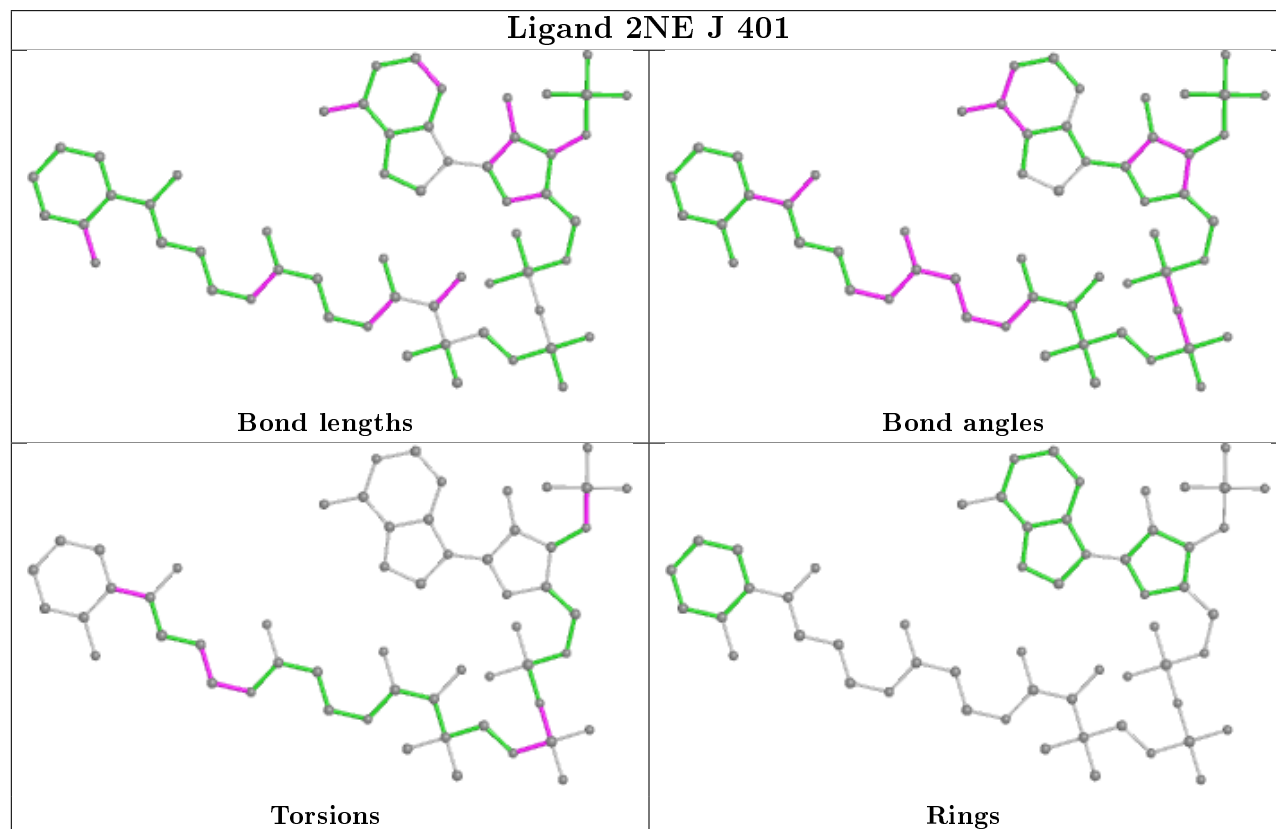
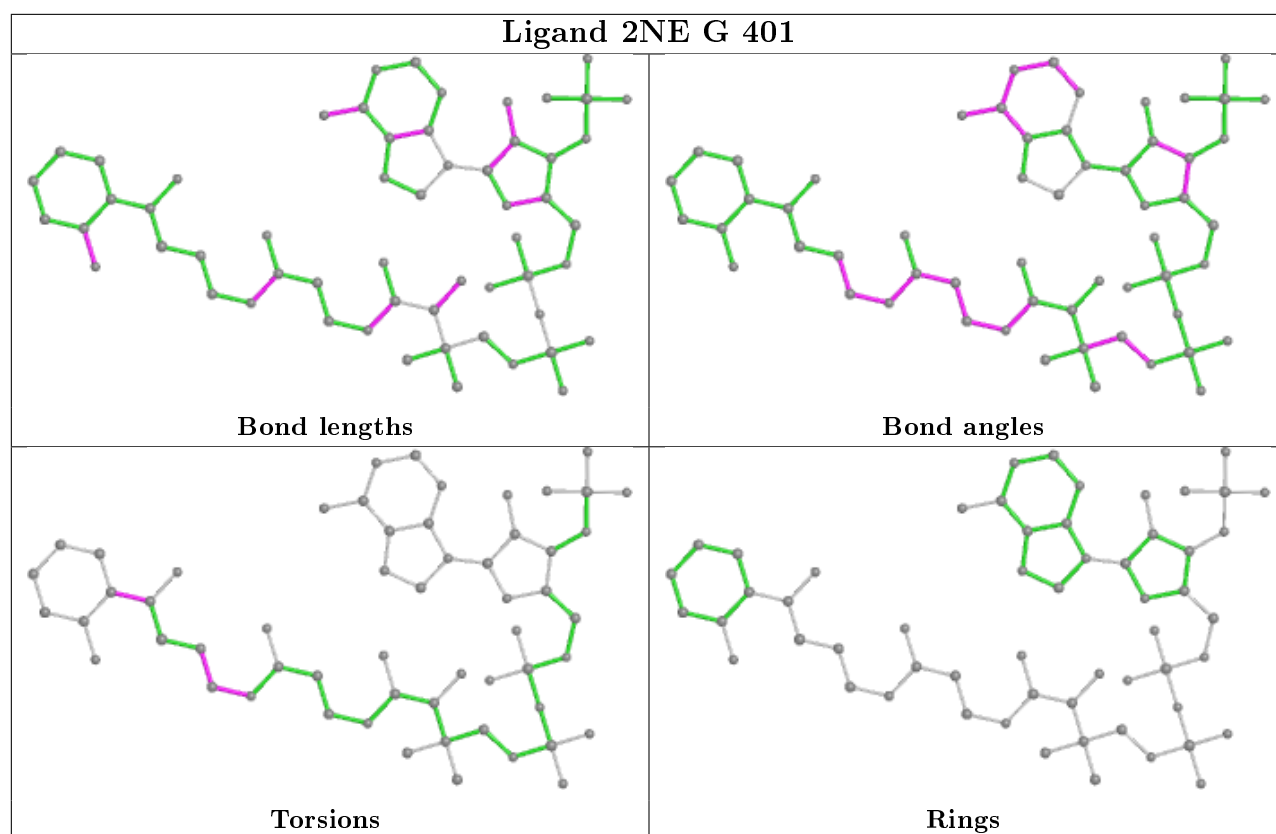
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

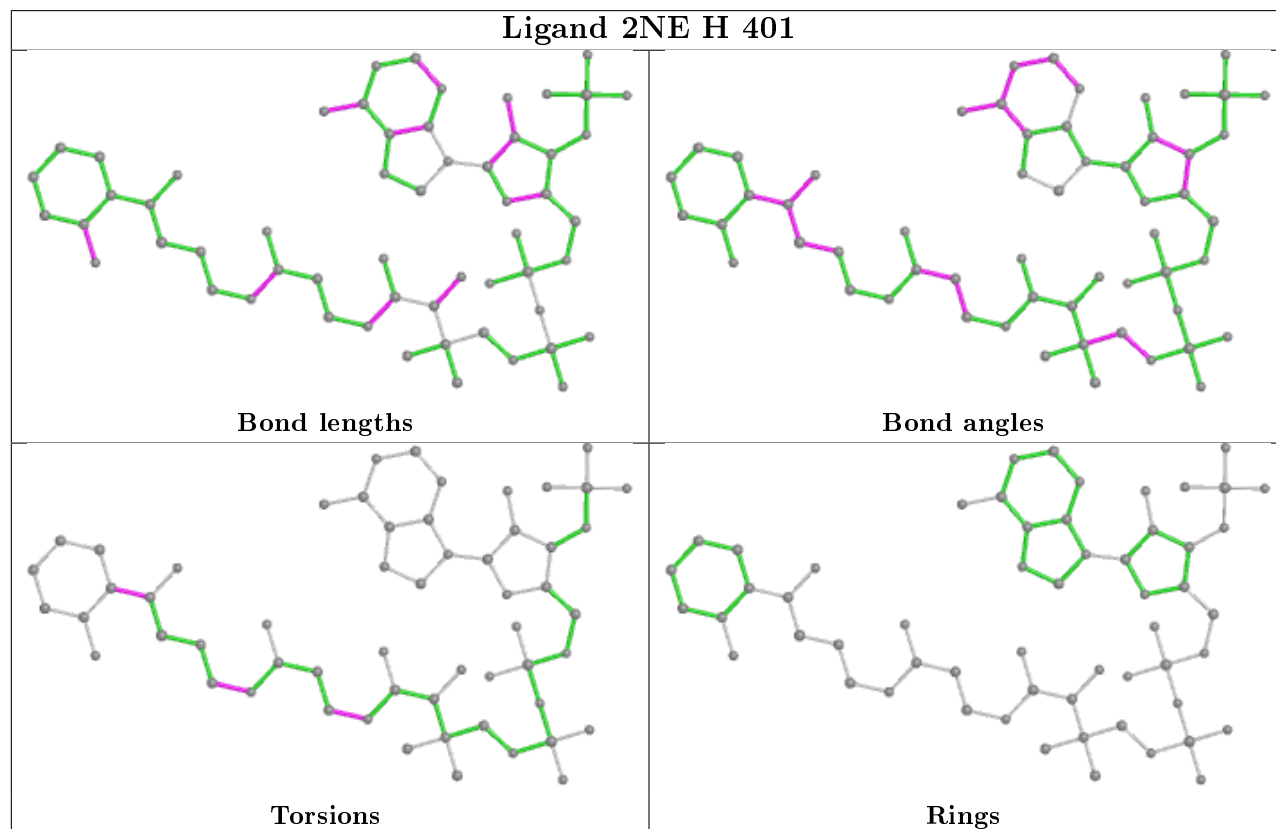
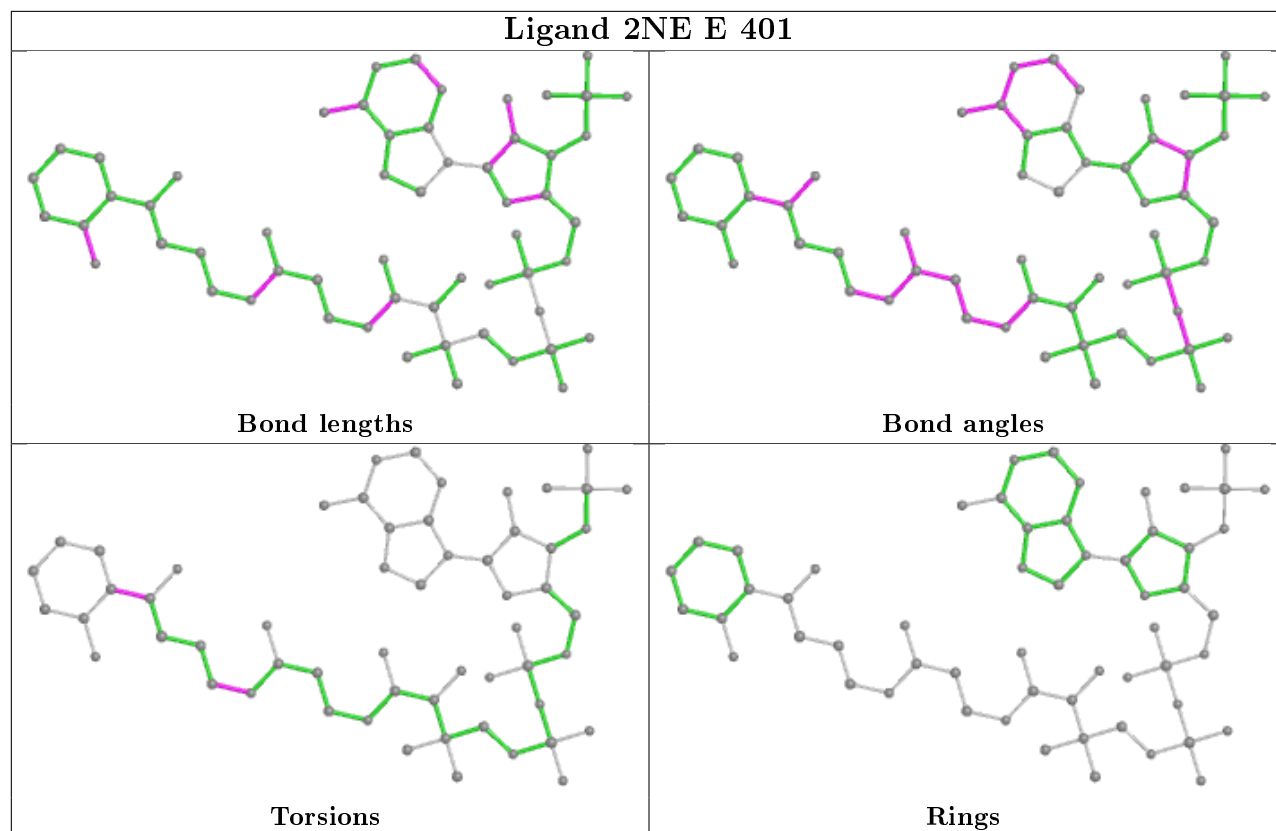
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



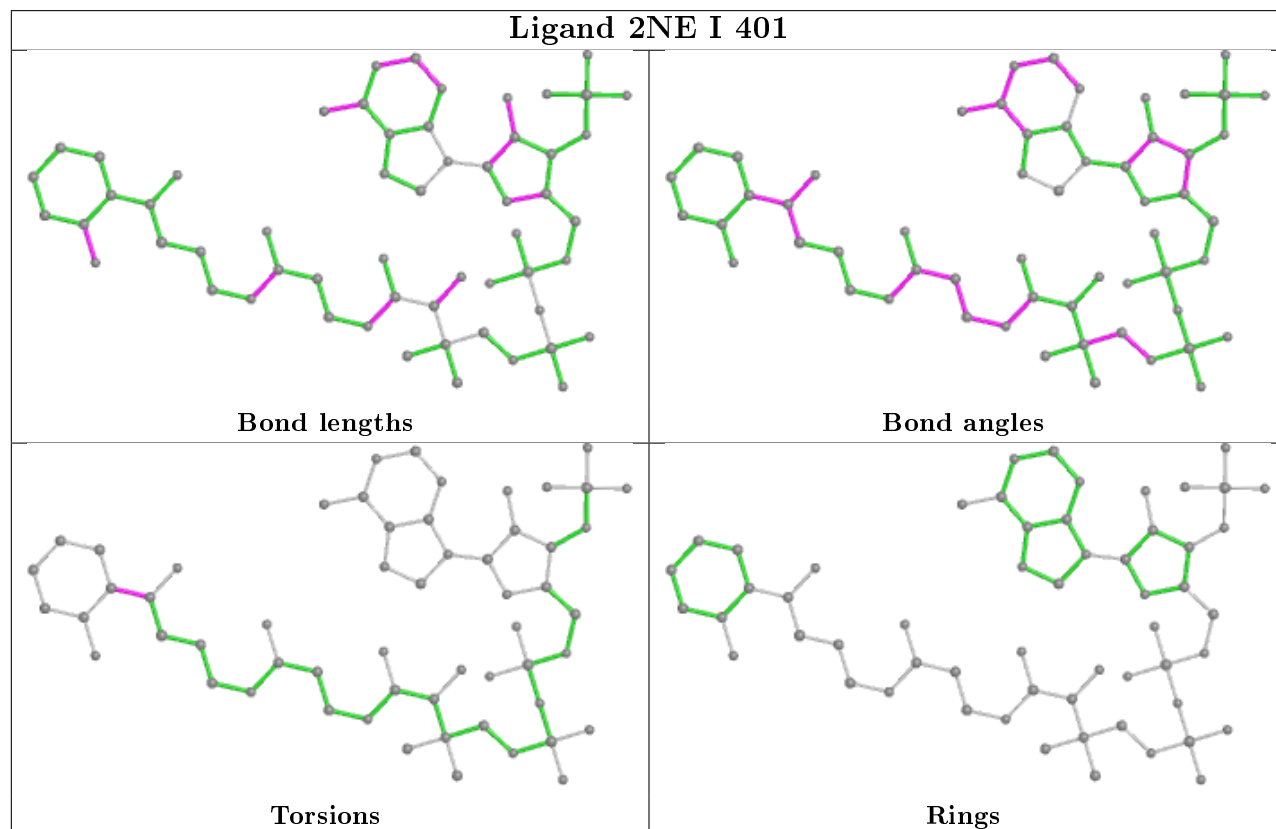
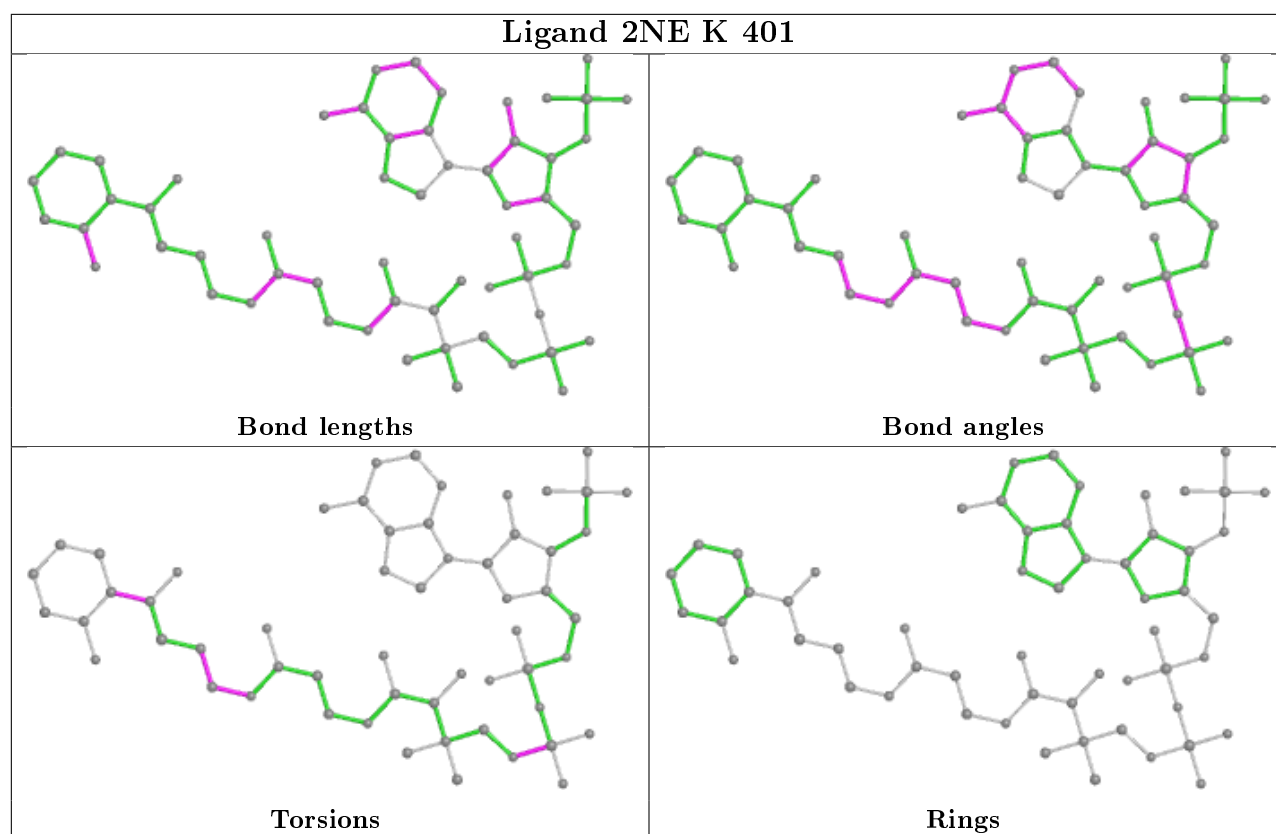


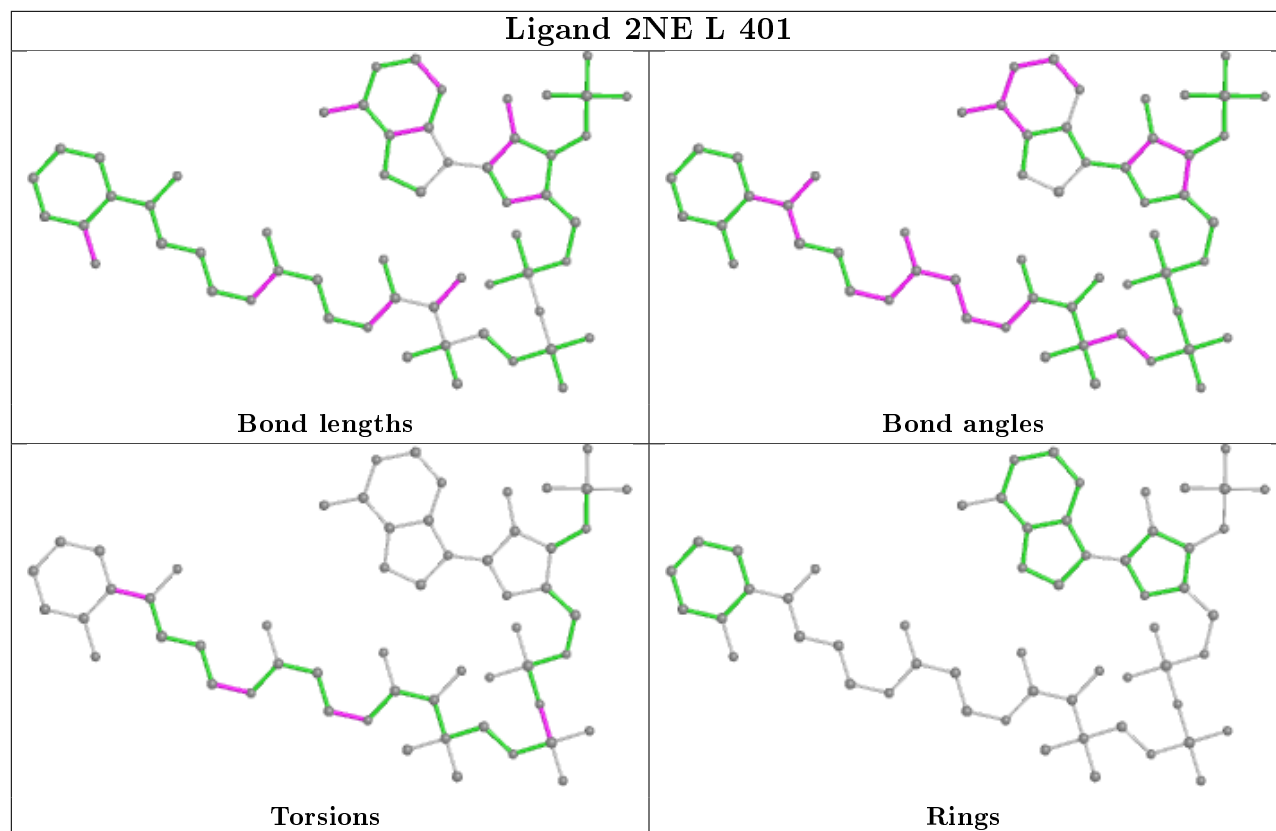












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	300/334 (89%)	-0.32	10 (3%) 46 44	7, 14, 28, 40	0
1	B	301/334 (90%)	-0.37	8 (2%) 54 53	8, 14, 30, 40	0
1	C	301/334 (90%)	-0.38	5 (1%) 70 71	8, 15, 29, 41	0
1	D	299/334 (89%)	-0.32	5 (1%) 70 71	9, 16, 28, 52	0
1	E	298/334 (89%)	-0.40	4 (1%) 77 78	9, 15, 28, 37	0
1	F	298/334 (89%)	-0.46	4 (1%) 77 78	9, 14, 26, 37	0
1	G	301/334 (90%)	-0.33	7 (2%) 60 60	8, 14, 27, 40	0
1	H	301/334 (90%)	-0.33	4 (1%) 77 78	9, 15, 26, 40	0
1	I	301/334 (90%)	-0.37	5 (1%) 70 71	9, 16, 28, 39	0
1	J	297/334 (88%)	-0.12	15 (5%) 28 25	11, 19, 33, 45	0
1	K	298/334 (89%)	-0.34	2 (0%) 87 88	11, 16, 29, 49	0
1	L	298/334 (89%)	-0.38	3 (1%) 82 83	10, 16, 28, 43	0
All	All	3593/4008 (89%)	-0.34	72 (2%) 65 65	7, 15, 29, 52	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	128	VAL	6.1
1	G	129	ALA	6.0
1	D	128	VAL	5.2
1	A	129	ALA	5.1
1	J	129	ALA	5.1
1	G	128	VAL	5.1
1	G	14	ALA	5.0
1	D	16	SER	4.8
1	C	14	ALA	4.8
1	A	102	CYS	4.6
1	B	14	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	I	129	ALA	4.6
1	H	129	ALA	4.5
1	C	128	VAL	4.5
1	B	128	VAL	4.4
1	H	128	VAL	4.0
1	A	128	VAL	3.9
1	I	14	ALA	3.9
1	J	32	ASP	3.8
1	A	152	CYS	3.6
1	A	169	CYS	3.6
1	C	129	ALA	3.5
1	J	268	LEU	3.5
1	D	17	ASP	3.3
1	F	268	LEU	3.2
1	K	17	ASP	3.2
1	J	125	THR	3.2
1	J	126	VAL	3.1
1	A	124	ASP	2.9
1	A	94	PRO	2.9
1	J	119	SER	2.9
1	D	268	LEU	2.9
1	J	120	GLY	2.8
1	E	128	VAL	2.8
1	D	129	ALA	2.8
1	F	17	ASP	2.7
1	K	32	ASP	2.7
1	G	268	LEU	2.7
1	G	124	ASP	2.6
1	J	33	ASP	2.6
1	J	94	PRO	2.6
1	B	124	ASP	2.6
1	C	124	ASP	2.6
1	H	268	LEU	2.6
1	J	97	GLY	2.5
1	L	17	ASP	2.5
1	I	32	ASP	2.5
1	C	268	LEU	2.4
1	B	129	ALA	2.4
1	E	304	PRO	2.3
1	F	29	ASP	2.3
1	F	32	ASP	2.3
1	I	268	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	32	ASP	2.3
1	J	124	ASP	2.3
1	G	32	ASP	2.3
1	J	98	GLY	2.2
1	A	165	LEU	2.2
1	J	96	ASP	2.2
1	A	127	ASP	2.2
1	B	29	ASP	2.2
1	I	128	VAL	2.2
1	G	127	ASP	2.2
1	J	123	ALA	2.2
1	A	268	LEU	2.1
1	E	17	ASP	2.1
1	L	32	ASP	2.1
1	B	123	ALA	2.1
1	H	95	LYS	2.1
1	E	268	LEU	2.0
1	L	268	LEU	2.0
1	B	33	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	2NE	A	401	57/57	0.83	0.21	15,29,95,103	0
3	PGE	G	402	10/10	0.84	0.20	12,36,54,55	0
3	PGE	B	402	10/10	0.86	0.22	8,36,65,68	0
3	PGE	J	402	10/10	0.87	0.17	16,34,42,43	0

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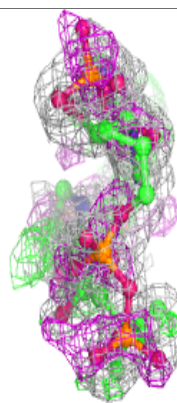
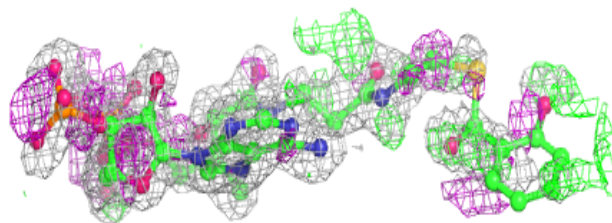
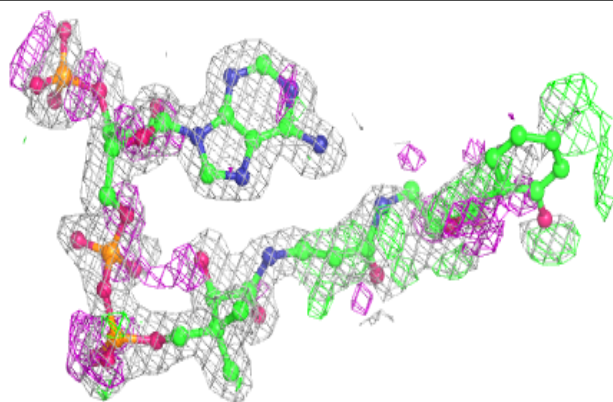
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2NE	J	401	57/57	0.87	0.20	20,31,84,130	0
2	2NE	D	401	57/57	0.90	0.14	15,24,73,81	0
3	PGE	D	402	10/10	0.91	0.18	9,37,62,67	0
2	2NE	K	401	57/57	0.91	0.15	11,22,92,117	0
2	2NE	I	401	57/57	0.91	0.13	12,19,103,109	0
2	2NE	H	401	57/57	0.92	0.14	13,20,78,113	0
2	2NE	B	401	57/57	0.93	0.12	13,21,82,123	0
2	2NE	L	401	57/57	0.93	0.12	12,22,94,96	0
2	2NE	F	401	57/57	0.94	0.10	10,18,76,113	0
2	2NE	G	401	57/57	0.94	0.11	12,17,79,105	0
2	2NE	C	401	57/57	0.94	0.11	12,19,95,117	0
2	2NE	E	401	57/57	0.94	0.10	10,16,78,104	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.

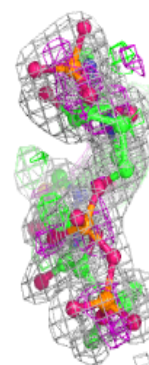
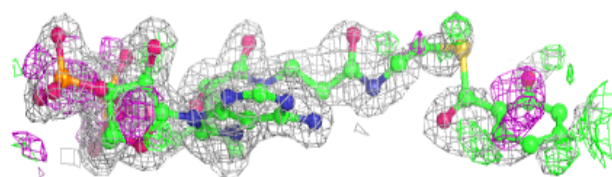
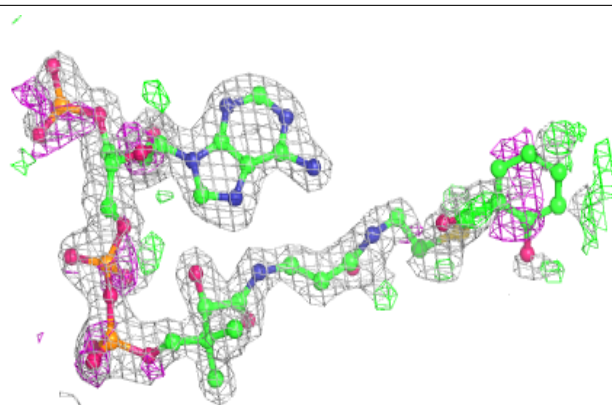
**Electron density around 2NE A 401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

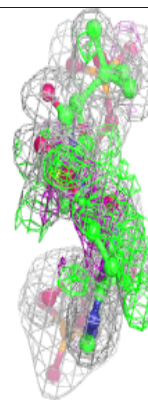
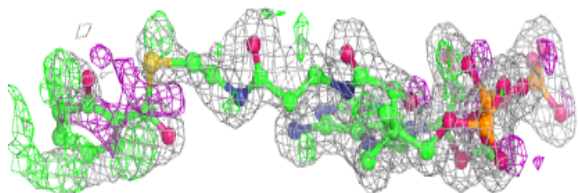
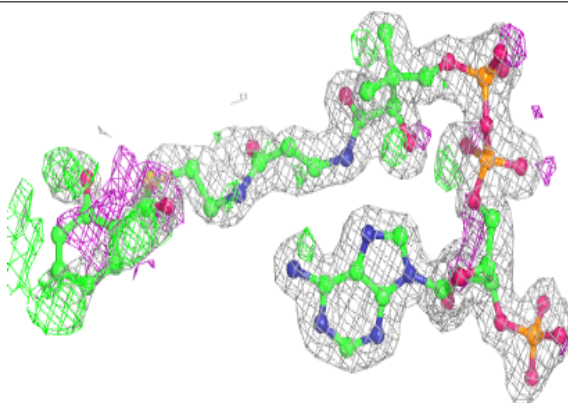


**Electron density around 2NE J 401:**

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

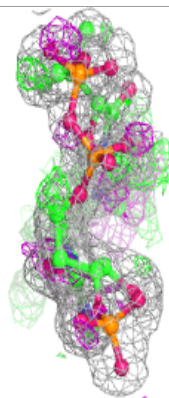
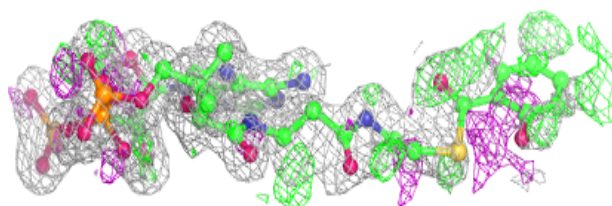
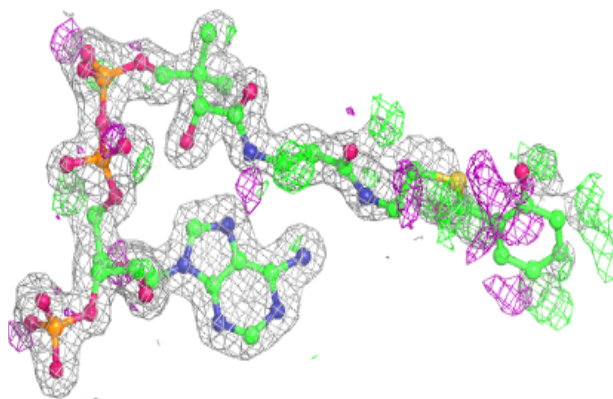
**Electron density around 2NE D 401:**

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

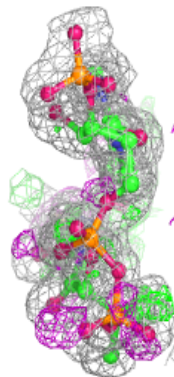
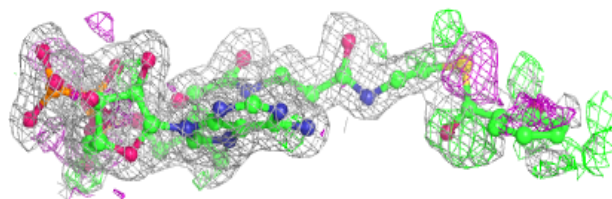
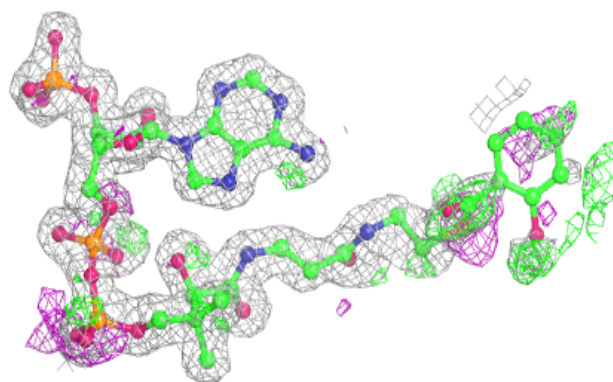


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and green (positive)

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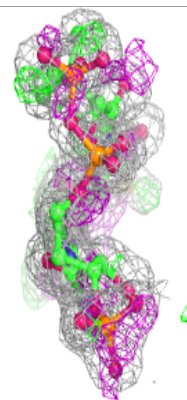
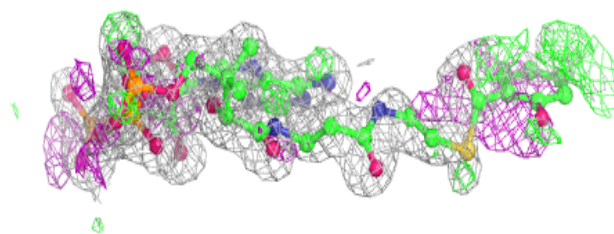
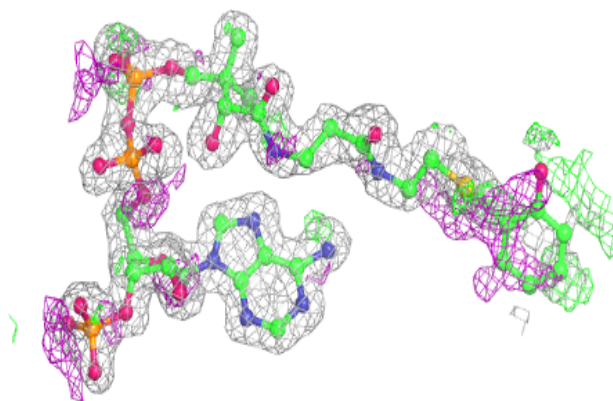
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



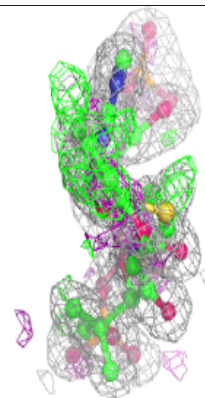
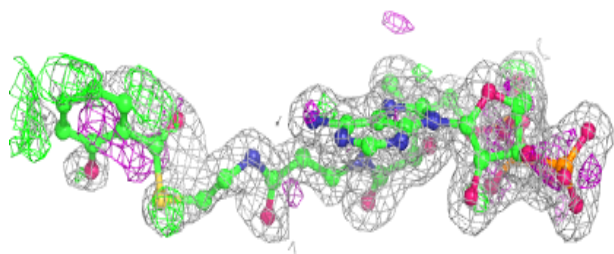
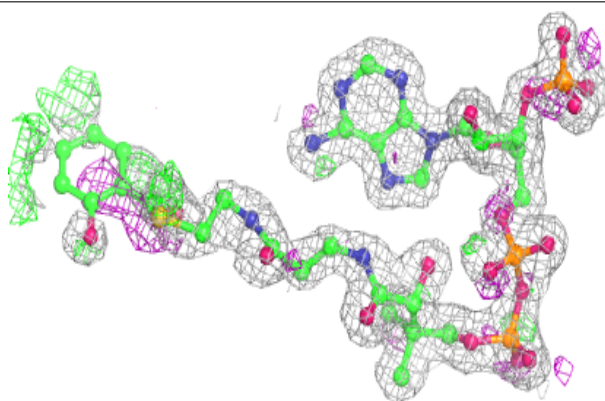


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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

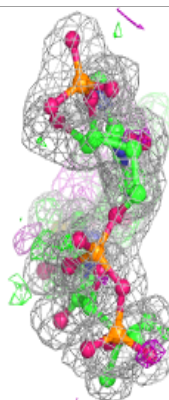
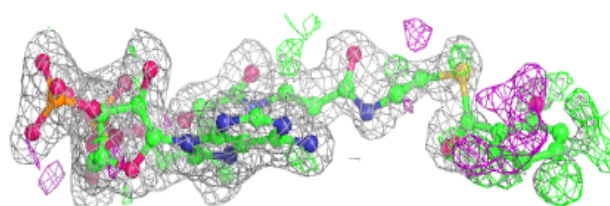
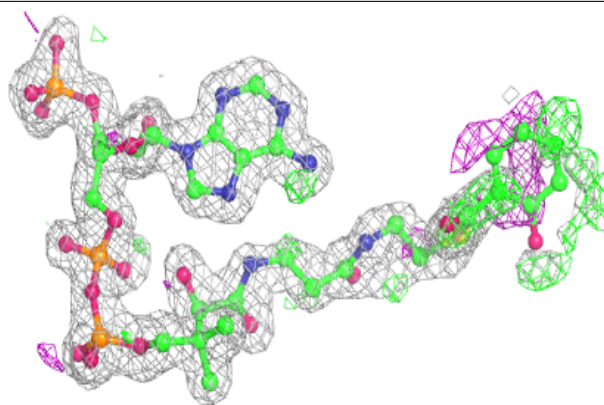
**Electron density around 2NE B 401:**

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and green (positive)

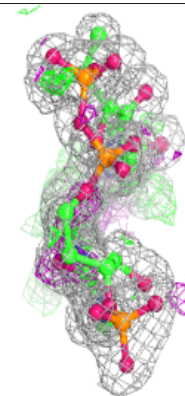
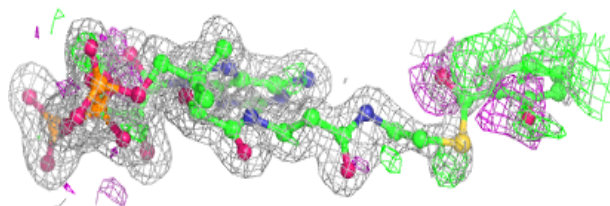
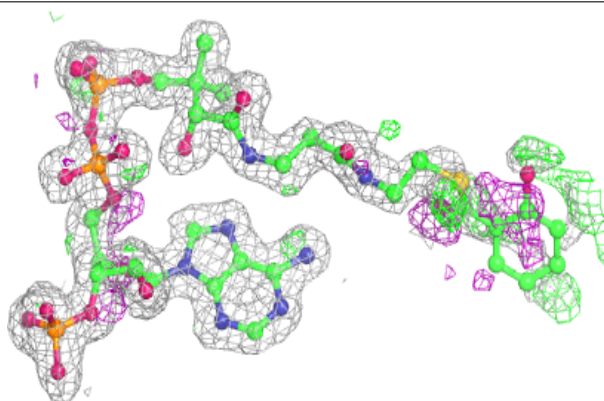


**Electron density around 2NE L 401:**

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and green (positive)

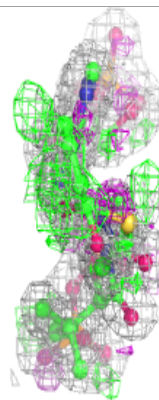
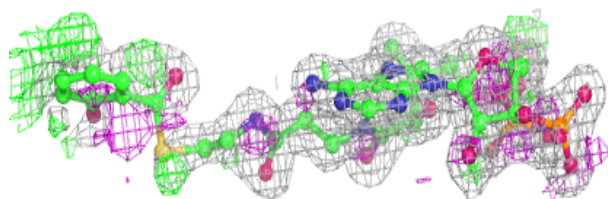
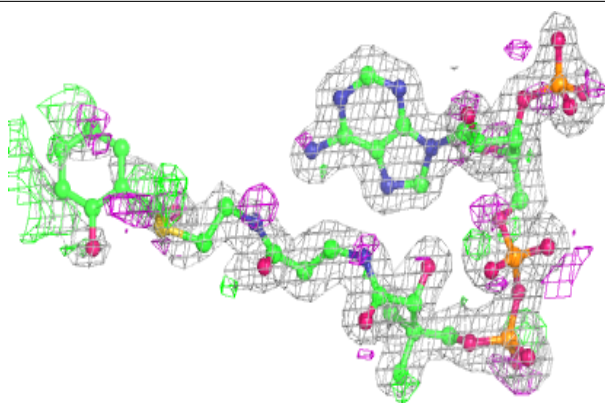
**Electron density around 2NE F 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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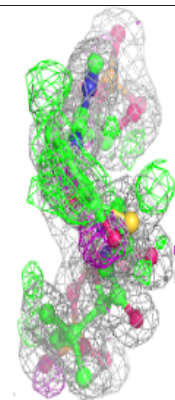
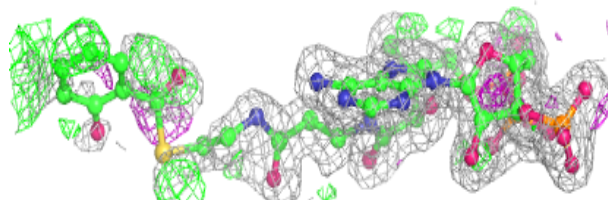
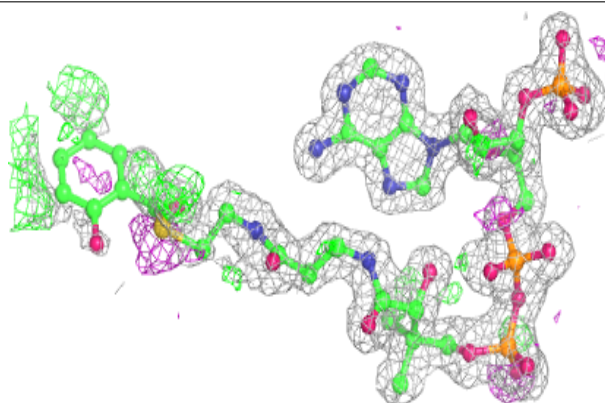


**Electron density around 2NE G 401:**

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and green (positive)

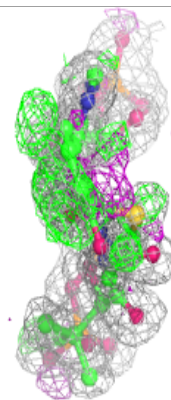
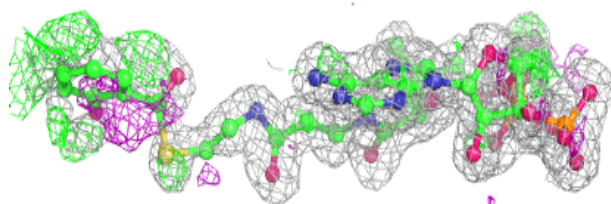
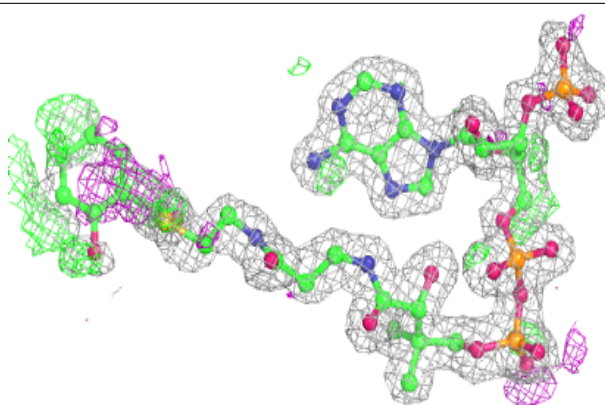
**Electron density around 2NE C 401:**

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



**Electron density around 2NE E 401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.