



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:41 AM UTC

PDB ID : 8VRE / pdb_00008vre
Title : Structure of PYCR1 complexed with NADH and N-formyl-L-proline
Authors : Tanner, J.J.; Meeks, K.R.
Deposited on : 2024-01-21
Resolution : 1.83 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

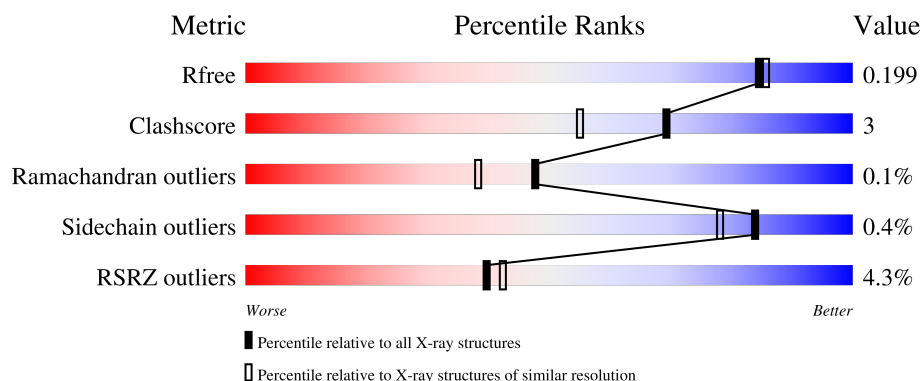
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	316	3% 82% 6% 12%
1	B	316	3% 84% • 12%
1	C	316	4% 78% 9% • 13%
1	D	316	5% 80% 7% 13%
1	E	316	4% 80% 7% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10695 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 Pyrroline-5-carboxylate reductase 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	4	0
			2006	1269	351	372	14			
1	B	278	Total	C	N	O	S	0	1	0
			1995	1258	352	373	12			
1	C	276	Total	C	N	O	S	0	1	0
			1950	1227	346	365	12			
1	D	276	Total	C	N	O	S	0	3	0
			1952	1232	343	365	12			
1	E	276	Total	C	N	O	S	0	2	0
			1958	1233	346	365	14			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP P32322
A	-20	HIS	-	expression tag	UNP P32322
A	-19	HIS	-	expression tag	UNP P32322
A	-18	HIS	-	expression tag	UNP P32322
A	-17	HIS	-	expression tag	UNP P32322
A	-16	HIS	-	expression tag	UNP P32322
A	-15	HIS	-	expression tag	UNP P32322
A	-14	SER	-	expression tag	UNP P32322
A	-13	SER	-	expression tag	UNP P32322
A	-12	GLY	-	expression tag	UNP P32322
A	-11	VAL	-	expression tag	UNP P32322
A	-10	ASP	-	expression tag	UNP P32322
A	-9	LEU	-	expression tag	UNP P32322
A	-8	GLY	-	expression tag	UNP P32322
A	-7	THR	-	expression tag	UNP P32322
A	-6	GLU	-	expression tag	UNP P32322
A	-5	ASN	-	expression tag	UNP P32322
A	-4	LEU	-	expression tag	UNP P32322
A	-3	TYR	-	expression tag	UNP P32322

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PHE	-	expression tag	UNP P32322
A	-1	GLN	-	expression tag	UNP P32322
A	0	SER	-	expression tag	UNP P32322
B	-21	MET	-	initiating methionine	UNP P32322
B	-20	HIS	-	expression tag	UNP P32322
B	-19	HIS	-	expression tag	UNP P32322
B	-18	HIS	-	expression tag	UNP P32322
B	-17	HIS	-	expression tag	UNP P32322
B	-16	HIS	-	expression tag	UNP P32322
B	-15	HIS	-	expression tag	UNP P32322
B	-14	SER	-	expression tag	UNP P32322
B	-13	SER	-	expression tag	UNP P32322
B	-12	GLY	-	expression tag	UNP P32322
B	-11	VAL	-	expression tag	UNP P32322
B	-10	ASP	-	expression tag	UNP P32322
B	-9	LEU	-	expression tag	UNP P32322
B	-8	GLY	-	expression tag	UNP P32322
B	-7	THR	-	expression tag	UNP P32322
B	-6	GLU	-	expression tag	UNP P32322
B	-5	ASN	-	expression tag	UNP P32322
B	-4	LEU	-	expression tag	UNP P32322
B	-3	TYR	-	expression tag	UNP P32322
B	-2	PHE	-	expression tag	UNP P32322
B	-1	GLN	-	expression tag	UNP P32322
B	0	SER	-	expression tag	UNP P32322
C	-21	MET	-	initiating methionine	UNP P32322
C	-20	HIS	-	expression tag	UNP P32322
C	-19	HIS	-	expression tag	UNP P32322
C	-18	HIS	-	expression tag	UNP P32322
C	-17	HIS	-	expression tag	UNP P32322
C	-16	HIS	-	expression tag	UNP P32322
C	-15	HIS	-	expression tag	UNP P32322
C	-14	SER	-	expression tag	UNP P32322
C	-13	SER	-	expression tag	UNP P32322
C	-12	GLY	-	expression tag	UNP P32322
C	-11	VAL	-	expression tag	UNP P32322
C	-10	ASP	-	expression tag	UNP P32322
C	-9	LEU	-	expression tag	UNP P32322
C	-8	GLY	-	expression tag	UNP P32322
C	-7	THR	-	expression tag	UNP P32322
C	-6	GLU	-	expression tag	UNP P32322
C	-5	ASN	-	expression tag	UNP P32322

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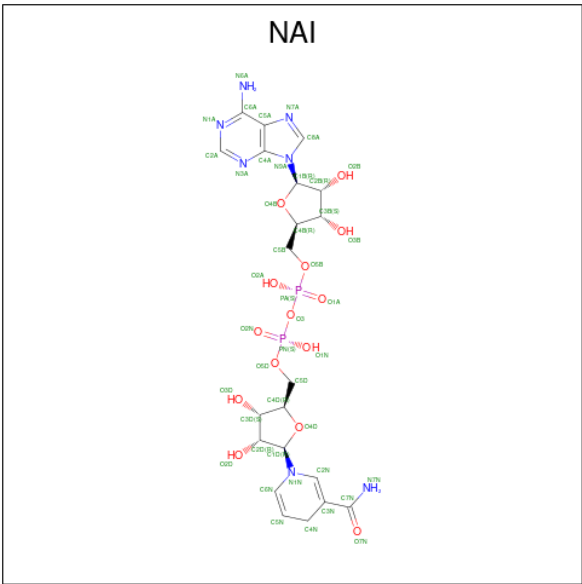
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	LEU	-	expression tag	UNP P32322
C	-3	TYR	-	expression tag	UNP P32322
C	-2	PHE	-	expression tag	UNP P32322
C	-1	GLN	-	expression tag	UNP P32322
C	0	SER	-	expression tag	UNP P32322
D	-21	MET	-	initiating methionine	UNP P32322
D	-20	HIS	-	expression tag	UNP P32322
D	-19	HIS	-	expression tag	UNP P32322
D	-18	HIS	-	expression tag	UNP P32322
D	-17	HIS	-	expression tag	UNP P32322
D	-16	HIS	-	expression tag	UNP P32322
D	-15	HIS	-	expression tag	UNP P32322
D	-14	SER	-	expression tag	UNP P32322
D	-13	SER	-	expression tag	UNP P32322
D	-12	GLY	-	expression tag	UNP P32322
D	-11	VAL	-	expression tag	UNP P32322
D	-10	ASP	-	expression tag	UNP P32322
D	-9	LEU	-	expression tag	UNP P32322
D	-8	GLY	-	expression tag	UNP P32322
D	-7	THR	-	expression tag	UNP P32322
D	-6	GLU	-	expression tag	UNP P32322
D	-5	ASN	-	expression tag	UNP P32322
D	-4	LEU	-	expression tag	UNP P32322
D	-3	TYR	-	expression tag	UNP P32322
D	-2	PHE	-	expression tag	UNP P32322
D	-1	GLN	-	expression tag	UNP P32322
D	0	SER	-	expression tag	UNP P32322
E	-21	MET	-	initiating methionine	UNP P32322
E	-20	HIS	-	expression tag	UNP P32322
E	-19	HIS	-	expression tag	UNP P32322
E	-18	HIS	-	expression tag	UNP P32322
E	-17	HIS	-	expression tag	UNP P32322
E	-16	HIS	-	expression tag	UNP P32322
E	-15	HIS	-	expression tag	UNP P32322
E	-14	SER	-	expression tag	UNP P32322
E	-13	SER	-	expression tag	UNP P32322
E	-12	GLY	-	expression tag	UNP P32322
E	-11	VAL	-	expression tag	UNP P32322
E	-10	ASP	-	expression tag	UNP P32322
E	-9	LEU	-	expression tag	UNP P32322
E	-8	GLY	-	expression tag	UNP P32322
E	-7	THR	-	expression tag	UNP P32322

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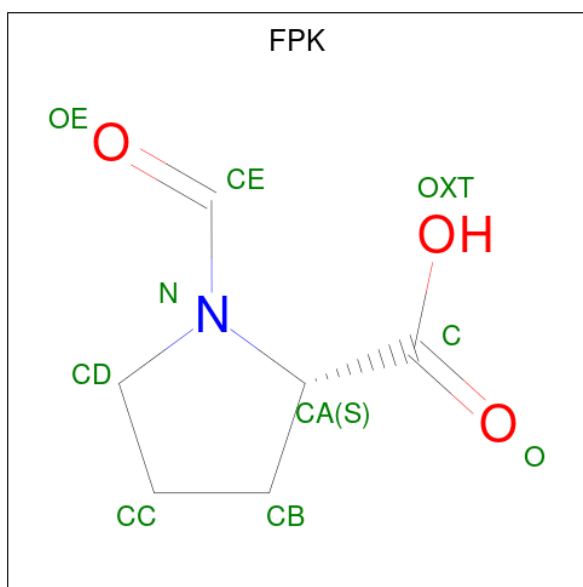
Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	GLU	-	expression tag	UNP P32322
E	-5	ASN	-	expression tag	UNP P32322
E	-4	LEU	-	expression tag	UNP P32322
E	-3	TYR	-	expression tag	UNP P32322
E	-2	PHE	-	expression tag	UNP P32322
E	-1	GLN	-	expression tag	UNP P32322
E	0	SER	-	expression tag	UNP P32322

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



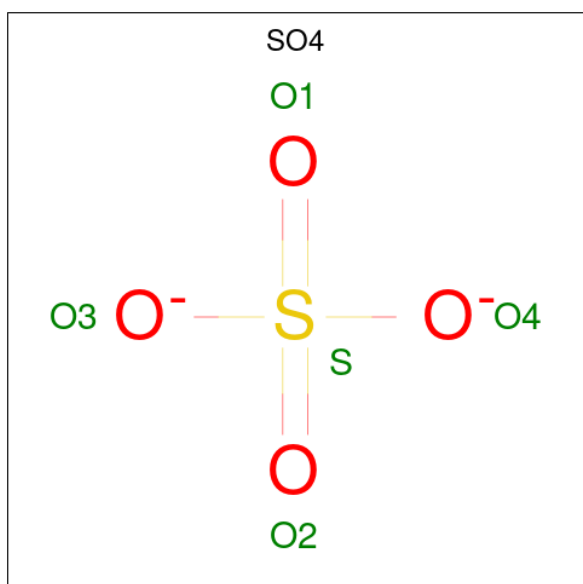
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 1-formyl-L-proline (CCD ID: FPK) (formula: C₆H₉NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	1	3		
3	B	1	Total	C	N	O	0	0
			10	6	1	3		
3	C	1	Total	C	N	O	0	0
			10	6	1	3		
3	D	1	Total	C	N	O	0	0
			10	6	1	3		
3	E	1	Total	C	N	O	0	0
			10	6	1	3		

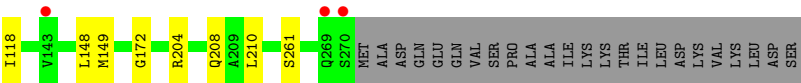
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



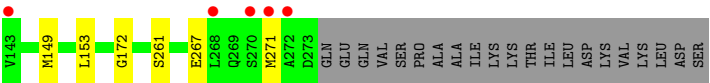
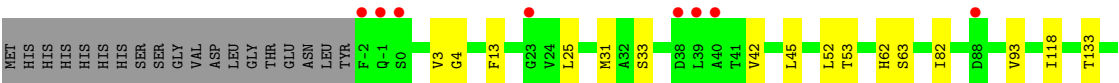
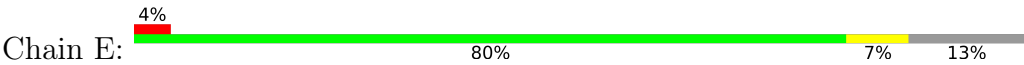
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total	O	0	0
			139	139		
5	B	115	Total	O	0	0
			115	115		
5	C	101	Total	O	0	0
			101	101		
5	D	92	Total	O	0	0
			92	92		
5	E	107	Total	O	0	0
			107	107		



● Molecule 1: Pyrroline-5-carboxylate reductase 1, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.53Å 179.29Å 88.36Å 90.00° 106.80° 90.00°	Depositor
Resolution (Å)	71.50 – 1.83 71.50 – 1.83	Depositor EDS
% Data completeness (in resolution range)	93.5 (71.50-1.83) 98.2 (71.50-1.83)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.83Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.175 , 0.202 0.173 , 0.199	Depositor DCC
R_{free} test set	6944 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10695	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: FPK, SO4, NAI

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	0.36	0/2049	0.55	0/2782
1	B	0.34	0/2031	0.54	0/2762
1	C	0.34	0/1983	0.54	0/2699
1	D	0.32	0/1992	0.49	0/2714
1	E	0.35	0/1994	0.55	0/2713
All	All	0.34	0/10049	0.54	0/13670

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

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	2006	0	2028	11	0
1	B	1995	0	1976	10	0
1	C	1950	0	1930	23	0
1	D	1952	0	1913	15	0
1	E	1958	0	1945	12	0
2	A	44	0	27	0	0
2	B	44	0	27	1	0
2	C	44	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	44	0	27	1	0
2	E	44	0	27	0	0
3	A	10	0	8	0	0
3	B	10	0	8	0	0
3	C	10	0	8	0	0
3	D	10	0	8	0	0
3	E	10	0	8	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	139	0	0	0	0
5	B	115	0	0	0	0
5	C	101	0	0	1	0
5	D	92	0	0	0	0
5	E	107	0	0	0	0
All	All	10695	0	9967	70	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:VAL:HG13	1:E:52:LEU:HD22	1.69	0.73
1:C:16:ALA:C	1:C:48:MET:HE1	2.21	0.64
1:C:99:VAL:HA	1:C:269:GLN:HG3	1.81	0.62
1:D:-3:TYR:HB3	1:D:148:LEU:HD13	1.81	0.62
1:D:63:SER:O	1:D:89:ARG:NH2	2.33	0.61
1:C:185:LEU:HD21	1:C:210:LEU:HD12	1.84	0.59
1:A:118:ILE:HD12	1:A:149[B]:MET:HG2	1.85	0.58
1:C:220:SER:OG	1:C:222:GLN:HG3	2.06	0.56
1:B:99:VAL:HA	1:B:269:GLN:NE2	2.21	0.56
1:E:267:GLU:HB3	1:E:271:MET:HE3	1.89	0.54
1:C:210:LEU:HB3	1:D:210:LEU:HD11	1.89	0.53
1:B:42:VAL:HG13	1:B:52:LEU:HD22	1.90	0.53
1:C:212:GLY:O	1:C:216:MET:HG3	2.09	0.53
1:C:264:ARG:HA	1:C:267:GLU:HG2	1.91	0.53
1:E:3:VAL:HG21	1:E:25:LEU:HD11	1.92	0.52
1:D:1:MET:HE3	1:D:3:VAL:HG23	1.92	0.51
1:C:57:LYS:O	1:C:61:GLN:HG3	2.11	0.50
1:A:220:SER:OG	1:A:222:GLN:HG3	2.11	0.50
1:C:93:VAL:HG21	1:C:149:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ILE:O	1:B:82:ILE:HG13	2.11	0.50
1:D:8:ALA:O	1:D:41:THR:OG1	2.29	0.49
1:A:93:VAL:HG21	1:A:149[B]:MET:HE2	1.94	0.49
1:D:24:VAL:HG23	1:D:25:LEU:HD12	1.93	0.49
1:C:37:MET:HG3	1:C:42:VAL:HG11	1.93	0.49
1:A:78:ILE:O	1:A:82:ILE:HG13	2.13	0.49
1:C:226:GLN:NE2	5:C:501:HOH:O	2.22	0.49
1:B:74:ILE:HG22	1:B:78:ILE:HG12	1.96	0.48
1:D:4:GLY:HA3	1:D:63:SER:OG	2.15	0.47
1:C:33:SER:HA	1:C:53:THR:O	2.14	0.47
1:B:44:ALA:O	1:B:48:MET:HG3	2.13	0.47
1:D:9:GLY:HA3	2:D:401:NAI:O5B	2.15	0.46
1:A:267:GLU:O	1:A:271:MET:HG3	2.15	0.46
1:C:16:ALA:O	1:C:48:MET:HE1	2.17	0.45
1:C:36:ASP:C	1:C:38:ASP:H	2.23	0.45
1:C:37:MET:HE1	1:C:53:THR:C	2.42	0.45
1:C:78:ILE:O	1:C:82:ILE:HG13	2.17	0.45
1:A:4:GLY:HA3	1:A:63[A]:SER:OG	2.16	0.44
1:C:204:ARG:HH12	1:C:208:GLN:HB2	1.82	0.44
1:D:1:MET:HE2	1:D:1:MET:HB3	1.86	0.44
1:B:267:GLU:C	1:B:269:GLN:H	2.25	0.44
1:B:9:GLY:HA3	2:B:401:NAI:O5B	2.18	0.44
1:C:216:MET:HE2	1:C:216:MET:HB3	1.93	0.43
1:D:118:ILE:HD13	1:D:149[B]:MET:HG2	2.00	0.43
1:D:80:ASP:OD2	1:D:107:LYS:HE3	2.19	0.43
1:B:81:GLU:HG2	1:B:82:ILE:HG23	2.00	0.42
1:D:60:VAL:HG21	1:D:82:ILE:HB	2.01	0.42
1:D:204:ARG:NH1	1:D:208:GLN:HB2	2.33	0.42
1:D:1:MET:HE1	1:D:25:LEU:HD11	2.02	0.42
1:E:82:ILE:C	1:E:82:ILE:HD12	2.43	0.42
1:E:93:VAL:HG21	1:E:149[B]:MET:HE2	2.01	0.42
1:C:231:VAL:HG12	1:C:238:THR:HG21	2.00	0.42
1:E:31:MET:HE3	1:E:62:HIS:HB3	2.00	0.42
1:C:37:MET:HE1	1:C:53:THR:CA	2.50	0.42
1:C:185:LEU:HA	1:C:185:LEU:HD23	1.86	0.42
1:A:74:ILE:HG22	1:A:78:ILE:HG12	2.01	0.42
1:B:33:SER:HA	1:B:53:THR:O	2.20	0.41
1:C:98:GLY:O	1:C:269:GLN:HG3	2.21	0.41
1:D:172:GLY:HA2	1:D:261:SER:OG	2.21	0.41
1:E:133:THR:HG21	1:E:153:LEU:HG	2.02	0.41
1:A:269:GLN:HA	1:A:269:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ARG:O	1:C:268:LEU:HD13	2.21	0.41
1:A:172:GLY:HA2	1:A:261:SER:OG	2.20	0.41
1:B:267:GLU:C	1:B:269:GLN:N	2.79	0.41
1:E:118:ILE:HD12	1:E:149[B]:MET:HG2	2.02	0.40
1:E:172:GLY:HA2	1:E:261:SER:OG	2.21	0.40
1:E:33:SER:HA	1:E:53:THR:O	2.22	0.40
1:A:149[B]:MET:HE1	1:A:152:LEU:HD23	2.02	0.40
1:E:4:GLY:HA3	1:E:63:SER:OG	2.22	0.40
1:A:33:SER:HA	1:A:53:THR:O	2.22	0.40
1:E:13:PHE:HA	1:E:45:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

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	280/316 (89%)	275 (98%)	5 (2%)	0	100	100
1	B	277/316 (88%)	270 (98%)	7 (2%)	0	100	100
1	C	275/316 (87%)	268 (98%)	6 (2%)	1 (0%)	30	18
1	D	277/316 (88%)	271 (98%)	6 (2%)	0	100	100
1	E	276/316 (87%)	271 (98%)	5 (2%)	0	100	100
All	All	1385/1580 (88%)	1355 (98%)	29 (2%)	1 (0%)	48	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	37	MET

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	205/251 (82%)	203 (99%)	2 (1%)	68	58
1	B	200/251 (80%)	200 (100%)	0	100	100
1	C	193/251 (77%)	191 (99%)	2 (1%)	68	58
1	D	191/251 (76%)	191 (100%)	0	100	100
1	E	195/251 (78%)	195 (100%)	0	100	100
All	All	984/1255 (78%)	980 (100%)	4 (0%)	84	78

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-4	LEU
1	A	78	ILE
1	C	268	LEU
1	C	269	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	219	HIS
1	A	226	GLN
1	B	269	GLN
1	C	28	HIS
1	C	62	HIS
1	C	226	GLN
1	C	269	GLN
1	D	222	GLN
1	E	62	HIS
1	E	222	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAI	D	401	-	47,48,48	1.49	10 (21%)	64,73,73	1.51	10 (15%)
2	NAI	E	401	-	47,48,48	1.36	5 (10%)	64,73,73	1.51	12 (18%)
4	SO4	A	403	-	4,4,4	0.27	0	6,6,6	0.09	0
3	FPK	A	402	-	10,10,10	1.20	1 (10%)	11,13,13	1.49	1 (9%)
4	SO4	B	403	-	4,4,4	0.32	0	6,6,6	0.09	0
2	NAI	B	401	-	47,48,48	1.40	7 (14%)	64,73,73	1.53	10 (15%)
3	FPK	C	402	-	10,10,10	1.24	1 (10%)	11,13,13	1.45	1 (9%)
3	FPK	D	402	-	10,10,10	1.19	1 (10%)	11,13,13	1.59	1 (9%)
2	NAI	A	401	-	47,48,48	1.41	8 (17%)	64,73,73	1.53	9 (14%)
2	NAI	C	401	-	47,48,48	1.39	7 (14%)	64,73,73	1.59	12 (18%)
3	FPK	E	402	-	10,10,10	1.22	1 (10%)	11,13,13	1.47	2 (18%)
3	FPK	B	402	-	10,10,10	1.11	1 (10%)	11,13,13	1.71	2 (18%)

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	NAI	D	401	-	-	4/29/72/72	0/5/5/5
2	NAI	E	401	-	-	4/29/72/72	0/5/5/5
3	FPK	A	402	-	-	0/5/16/16	0/1/1/1
2	NAI	B	401	-	-	4/29/72/72	0/5/5/5
3	FPK	C	402	-	-	0/5/16/16	0/1/1/1
3	FPK	D	402	-	-	0/5/16/16	0/1/1/1
2	NAI	A	401	-	-	3/29/72/72	0/5/5/5
2	NAI	C	401	-	-	4/29/72/72	0/5/5/5
3	FPK	E	402	-	-	0/5/16/16	0/1/1/1
3	FPK	B	402	-	-	0/5/16/16	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAI	PN-O3	3.95	1.63	1.59
2	B	401	NAI	PA-O3	3.93	1.63	1.59
2	C	401	NAI	PN-O5D	3.48	1.73	1.59
2	D	401	NAI	PN-O5D	3.46	1.72	1.59
2	E	401	NAI	PA-O5B	3.40	1.72	1.59
2	A	401	NAI	PA-O5B	3.37	1.72	1.59
2	C	401	NAI	PA-O5B	3.29	1.72	1.59
2	E	401	NAI	C8A-N9A	3.20	1.43	1.37
2	D	401	NAI	C8A-N9A	3.20	1.43	1.37
2	E	401	NAI	PN-O5D	3.14	1.71	1.59
2	D	401	NAI	PN-O3	3.14	1.62	1.59
2	C	401	NAI	C8A-N9A	3.10	1.42	1.37
2	D	401	NAI	PA-O5B	3.06	1.71	1.59
2	B	401	NAI	PA-O5B	3.02	1.71	1.59
3	E	402	FPK	CA-C	3.00	1.58	1.52
2	E	401	NAI	PN-O3	2.89	1.62	1.59
2	B	401	NAI	C8A-N9A	2.88	1.42	1.37
2	B	401	NAI	PN-O5D	2.77	1.70	1.59
2	A	401	NAI	C8A-N9A	2.76	1.42	1.37
3	C	402	FPK	CA-C	2.51	1.57	1.52
3	A	402	FPK	CA-C	2.43	1.57	1.52
3	D	402	FPK	CA-C	2.42	1.57	1.52
2	D	401	NAI	C2A-N1A	2.38	1.38	1.33
2	C	401	NAI	C3D-C4D	2.37	1.59	1.53
3	B	402	FPK	CA-C	2.36	1.57	1.52
2	A	401	NAI	PN-O5D	2.36	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAI	C8A-N7A	2.34	1.36	1.31
2	D	401	NAI	C4A-N3A	2.29	1.38	1.34
2	D	401	NAI	C5A-C4A	2.25	1.43	1.39
2	B	401	NAI	PN-O3	2.21	1.61	1.59
2	E	401	NAI	C3B-C4B	2.21	1.58	1.53
2	B	401	NAI	C3D-C4D	2.19	1.58	1.53
2	A	401	NAI	PA-O3	2.15	1.61	1.59
2	A	401	NAI	C4A-N3A	2.13	1.38	1.34
2	D	401	NAI	C8A-N7A	2.12	1.35	1.31
2	C	401	NAI	C7N-N7N	2.10	1.39	1.33
2	D	401	NAI	O5D-C5D	-2.08	1.36	1.44
2	C	401	NAI	O5D-C5D	-2.06	1.36	1.44
2	A	401	NAI	C7N-N7N	2.04	1.39	1.33
2	D	401	NAI	C7N-N7N	2.03	1.39	1.33
2	B	401	NAI	C2A-N1A	2.02	1.37	1.33
2	C	401	NAI	C4A-N3A	2.01	1.38	1.34

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAI	O2A-PA-O3	4.65	119.85	107.27
3	D	402	FPK	CB-CA-N	4.56	107.05	102.00
3	B	402	FPK	CB-CA-N	4.51	106.98	102.00
3	C	402	FPK	CB-CA-N	4.45	106.92	102.00
2	C	401	NAI	O2A-PA-O3	4.35	119.03	107.27
2	B	401	NAI	O2A-PA-O3	4.32	118.95	107.27
2	B	401	NAI	O1N-PN-O3	4.29	118.87	107.27
2	D	401	NAI	O2A-PA-O3	4.25	118.76	107.27
3	A	402	FPK	CB-CA-N	4.15	106.59	102.00
2	A	401	NAI	O1N-PN-O3	4.04	118.20	107.27
2	E	401	NAI	O2A-PA-O3	4.02	118.13	107.27
2	C	401	NAI	O1N-PN-O3	4.00	118.08	107.27
2	C	401	NAI	O3-PA-O1A	-3.96	98.78	110.70
2	E	401	NAI	O3-PA-O1A	-3.86	99.11	110.70
2	E	401	NAI	O1N-PN-O3	3.78	117.48	107.27
2	B	401	NAI	O3-PA-O1A	-3.76	99.41	110.70
2	A	401	NAI	O3-PA-O1A	-3.71	99.55	110.70
2	D	401	NAI	O3-PA-O1A	-3.68	99.63	110.70
3	E	402	FPK	CB-CA-N	3.56	105.93	102.00
2	D	401	NAI	O1N-PN-O3	3.37	116.39	107.27
2	C	401	NAI	O2A-PA-O1A	3.25	127.58	112.44
2	D	401	NAI	O2A-PA-O1A	3.20	127.33	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	NAI	O2A-PA-O1A	3.06	126.66	112.44
2	A	401	NAI	O2A-PA-O1A	3.02	126.50	112.44
2	B	401	NAI	O2A-PA-O1A	3.00	126.40	112.44
2	D	401	NAI	O1N-PN-O2N	2.62	124.63	112.44
2	C	401	NAI	O7N-C7N-N7N	-2.60	117.06	122.89
2	D	401	NAI	O7N-C7N-N7N	-2.58	117.10	122.89
2	E	401	NAI	O7N-C7N-N7N	-2.45	117.40	122.89
2	B	401	NAI	O1N-PN-O2N	2.40	123.59	112.44
2	A	401	NAI	O1N-PN-O2N	2.39	123.58	112.44
2	E	401	NAI	O1N-PN-O2N	2.34	123.34	112.44
2	D	401	NAI	O5B-PA-O1A	-2.33	99.70	108.94
2	E	401	NAI	C5B-C4B-C3B	-2.32	106.85	115.21
2	D	401	NAI	PA-O5B-C5B	-2.32	108.07	121.35
2	D	401	NAI	C5B-C4B-C3B	-2.31	106.88	115.21
2	C	401	NAI	O1N-PN-O2N	2.31	123.17	112.44
3	E	402	FPK	C-CA-N	2.29	117.25	112.50
2	B	401	NAI	C5B-C4B-C3B	-2.29	106.98	115.21
2	C	401	NAI	PA-O5B-C5B	-2.25	108.44	121.35
2	D	401	NAI	C4B-O4B-C1B	-2.25	104.51	109.47
2	C	401	NAI	C5B-C4B-C3B	-2.24	107.16	115.21
2	B	401	NAI	O7N-C7N-N7N	-2.23	117.89	122.89
2	A	401	NAI	C5B-C4B-C3B	-2.22	107.22	115.21
2	E	401	NAI	C4B-O4B-C1B	-2.20	104.61	109.47
2	C	401	NAI	C2A-N1A-C6A	-2.20	115.12	118.73
2	B	401	NAI	PA-O5B-C5B	-2.19	108.78	121.35
2	E	401	NAI	PA-O5B-C5B	-2.15	109.01	121.35
2	B	401	NAI	C3N-C2N-N1N	-2.15	120.05	123.20
2	A	401	NAI	O7N-C7N-N7N	-2.13	118.12	122.89
2	E	401	NAI	C4A-N9A-C1B	-2.12	121.68	126.63
2	C	401	NAI	C4B-O4B-C1B	-2.09	104.84	109.47
2	E	401	NAI	N9A-C8A-N7A	-2.08	110.98	113.94
2	C	401	NAI	O4B-C1B-C2B	-2.08	102.17	106.62
2	A	401	NAI	C4A-N9A-C1B	-2.07	121.78	126.63
2	C	401	NAI	O5D-PN-O2N	-2.06	100.75	108.94
2	A	401	NAI	C3B-C2B-C1B	-2.04	97.61	101.46
2	E	401	NAI	C4A-N9A-C8A	2.02	107.86	105.74
3	B	402	FPK	O-C-CA	-2.01	116.26	122.44
2	B	401	NAI	C4B-O4B-C1B	-2.01	105.03	109.47

There are no chirality outliers.

All (19) torsion outliers are listed below:

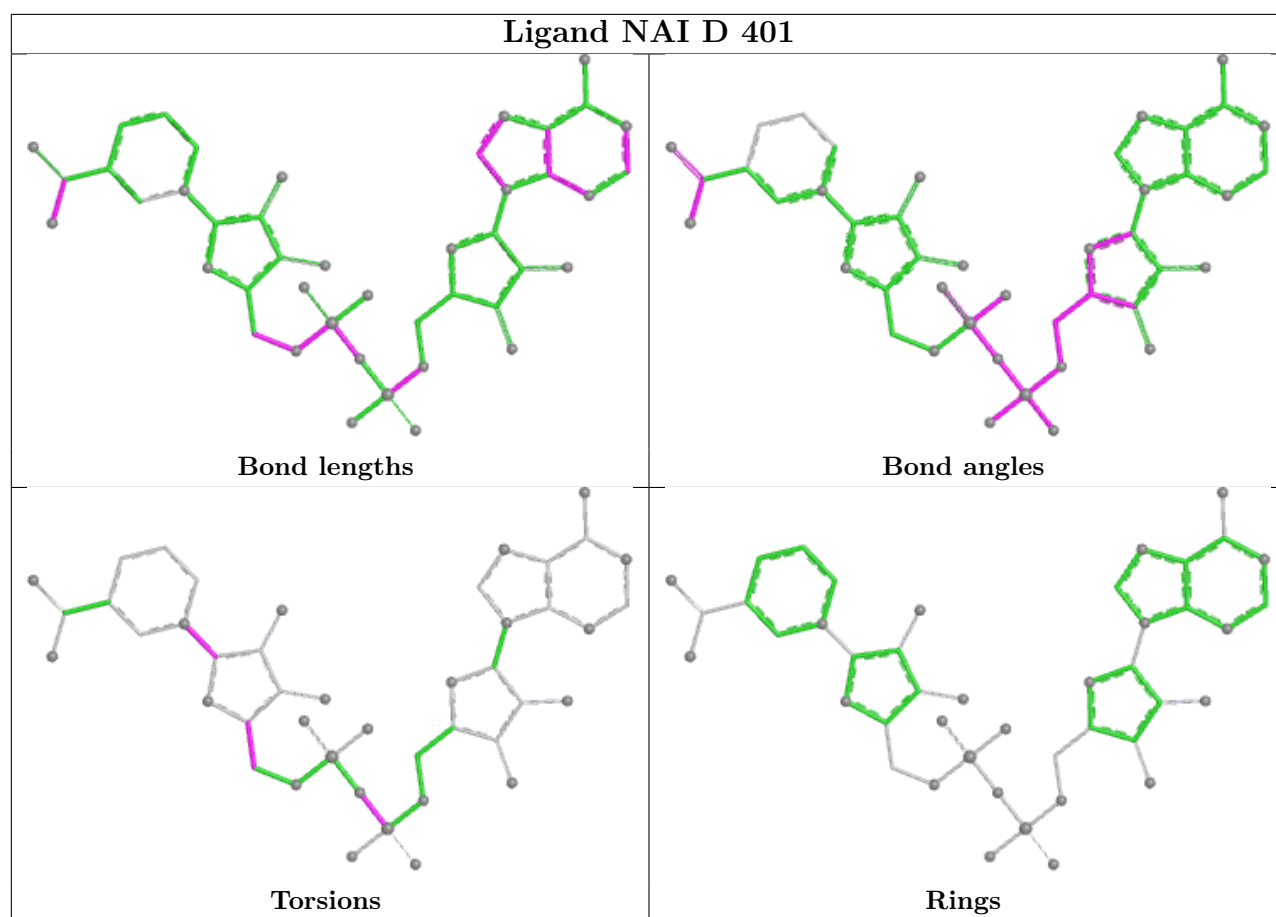
Mol	Chain	Res	Type	Atoms
2	C	401	NAI	C2B-C1B-N9A-C8A
2	A	401	NAI	C2B-C1B-N9A-C8A
2	A	401	NAI	O4D-C1D-N1N-C6N
2	C	401	NAI	O4D-C1D-N1N-C6N
2	B	401	NAI	O4D-C1D-N1N-C6N
2	E	401	NAI	O4D-C1D-N1N-C6N
2	D	401	NAI	O4D-C1D-N1N-C6N
2	D	401	NAI	O4D-C4D-C5D-O5D
2	D	401	NAI	C2D-C1D-N1N-C6N
2	B	401	NAI	C2B-C1B-N9A-C8A
2	E	401	NAI	C2B-C1B-N9A-C8A
2	A	401	NAI	PN-O3-PA-O2A
2	B	401	NAI	PN-O3-PA-O2A
2	C	401	NAI	PN-O3-PA-O2A
2	D	401	NAI	PN-O3-PA-O2A
2	E	401	NAI	PN-O3-PA-O2A
2	B	401	NAI	C2D-C1D-N1N-C6N
2	C	401	NAI	C2D-C1D-N1N-C6N
2	E	401	NAI	C2D-C1D-N1N-C6N

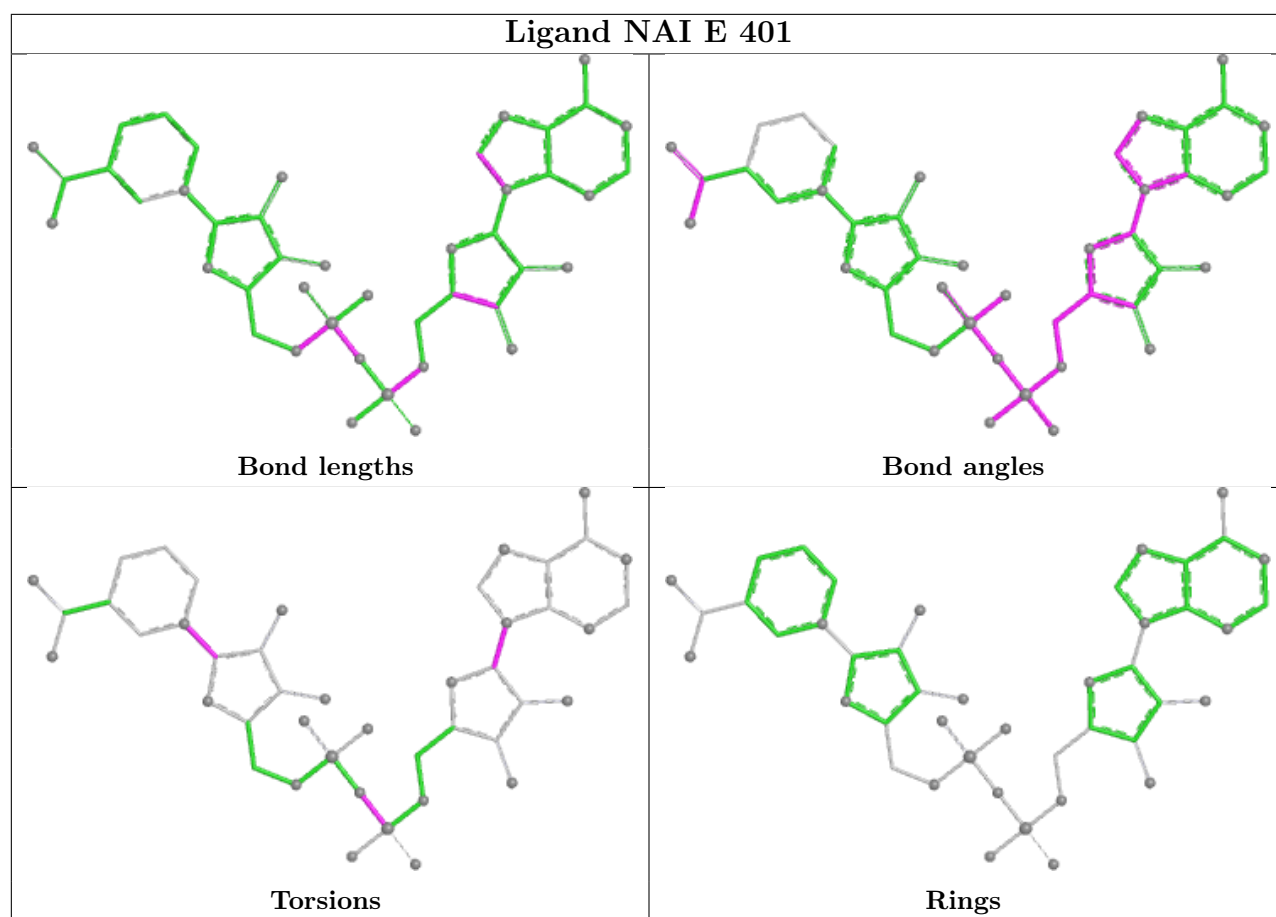
There are no ring outliers.

2 monomers are involved in 2 short contacts:

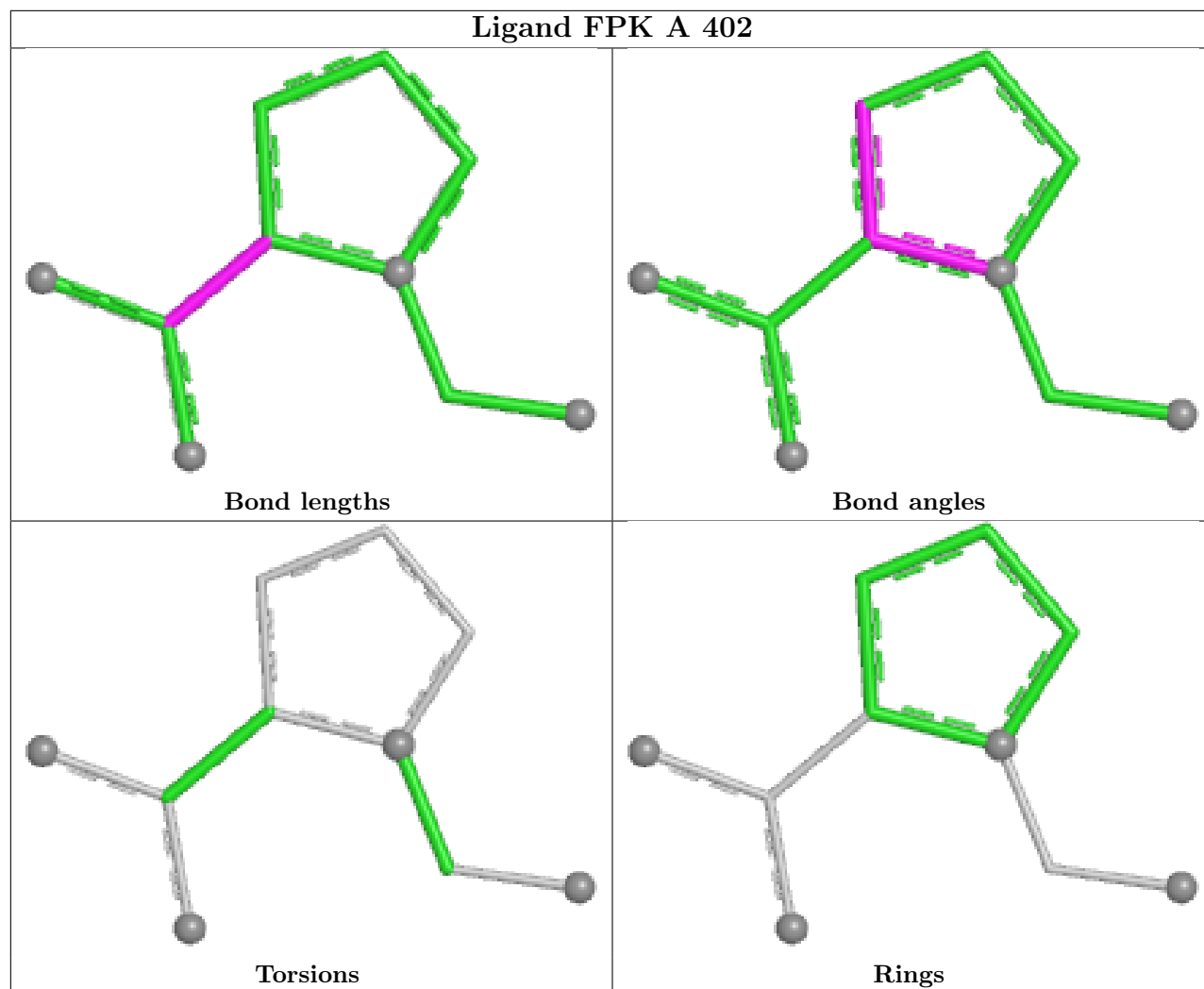
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	NAI	1	0
2	B	401	NAI	1	0

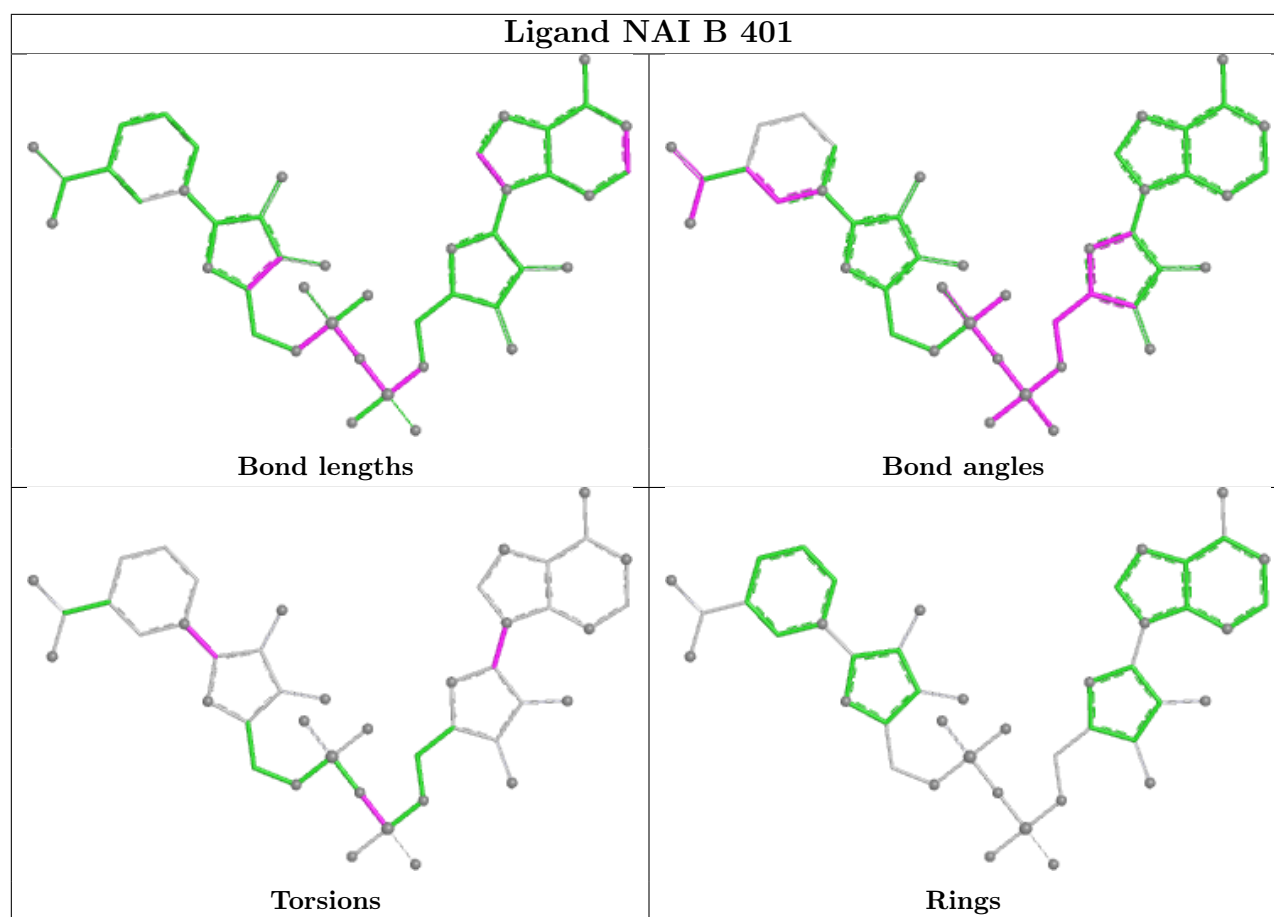
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



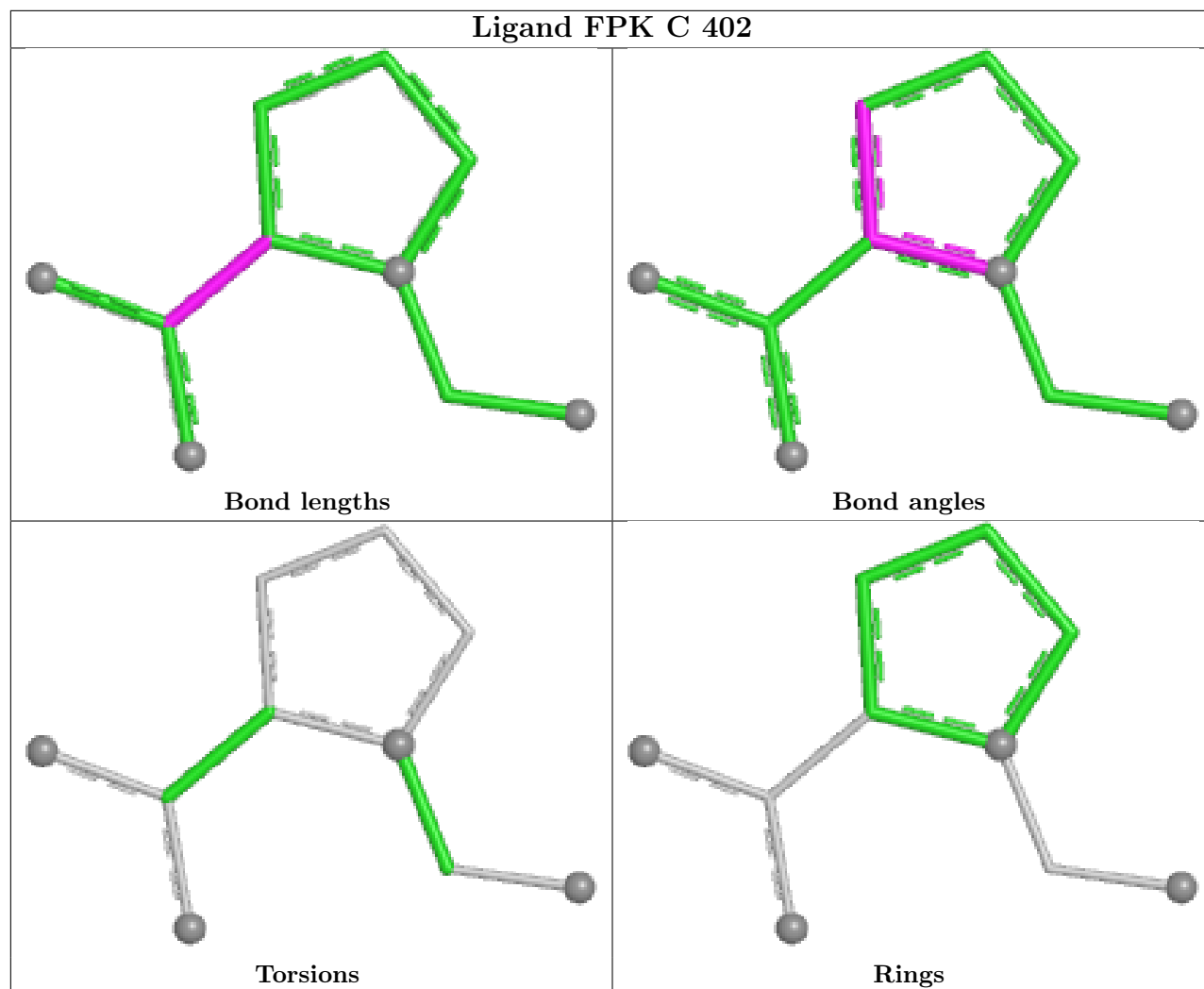


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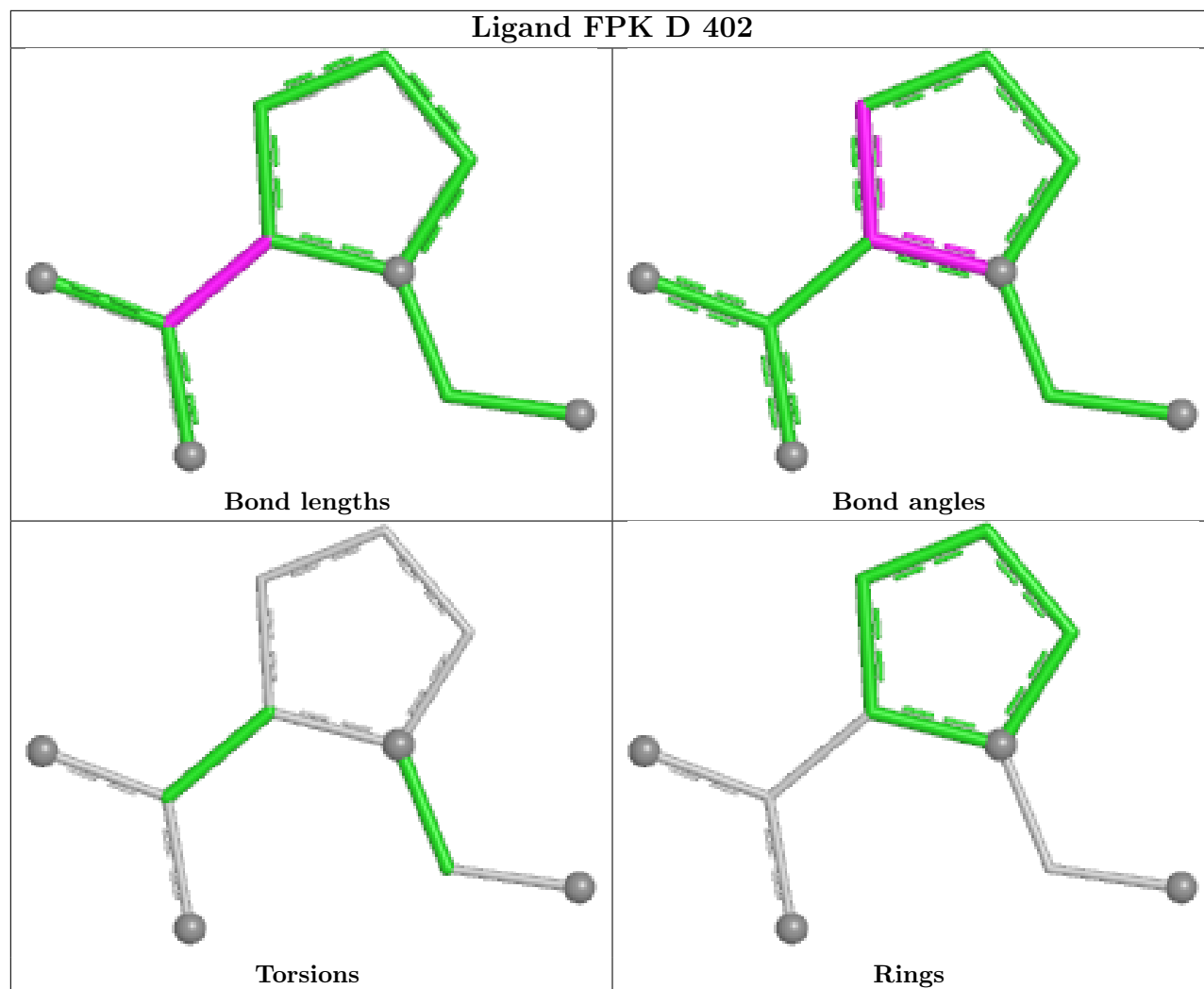


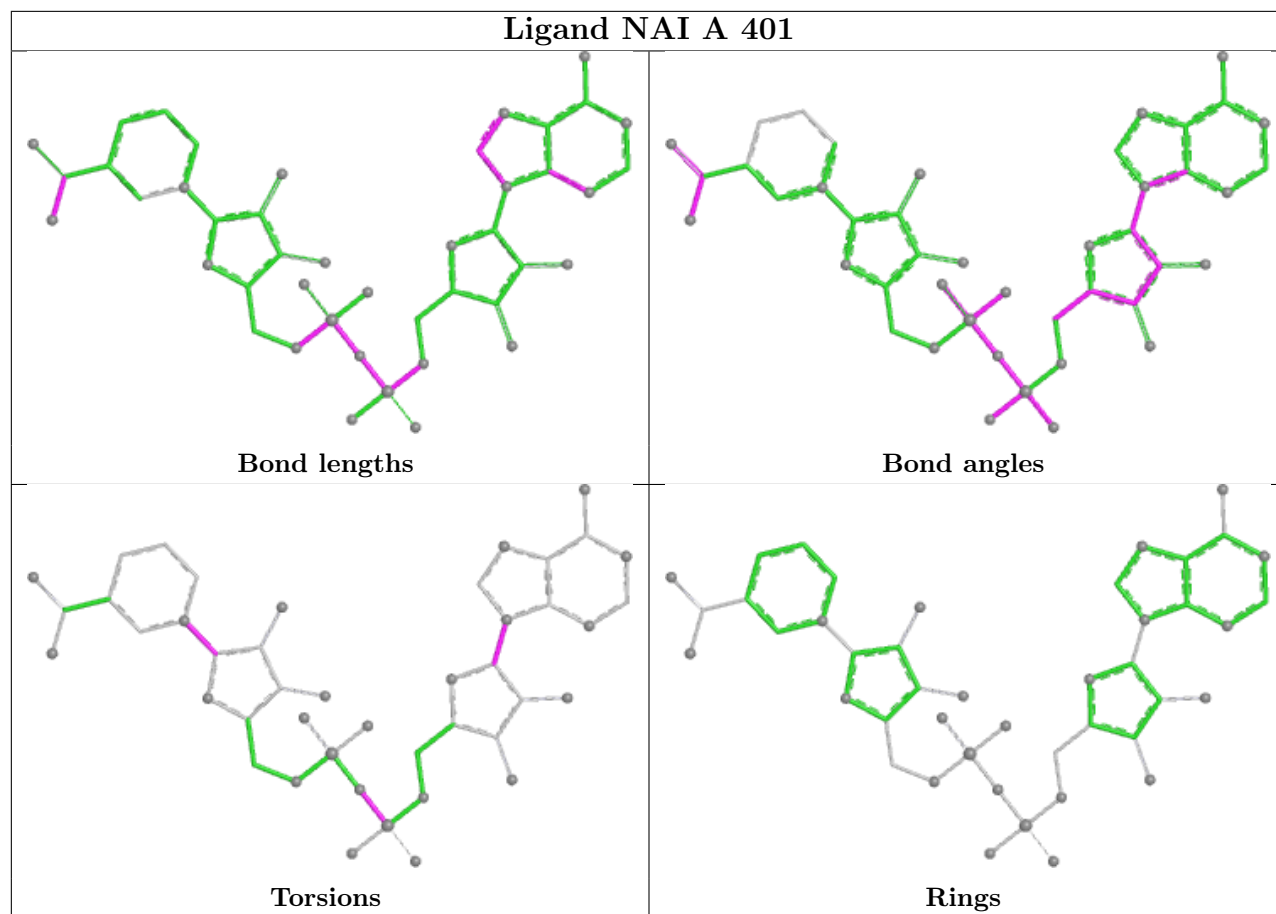


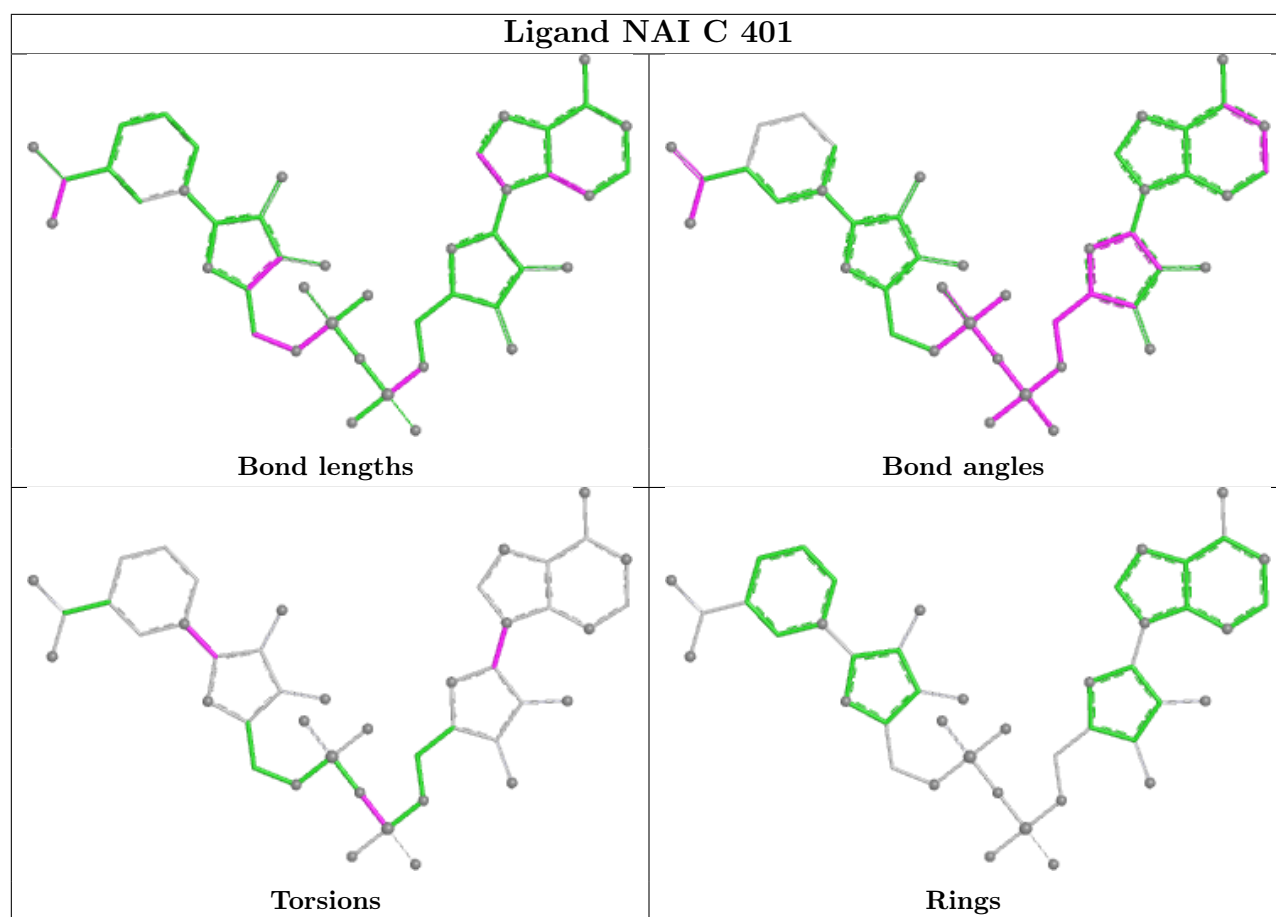
Ligand FPK C 402



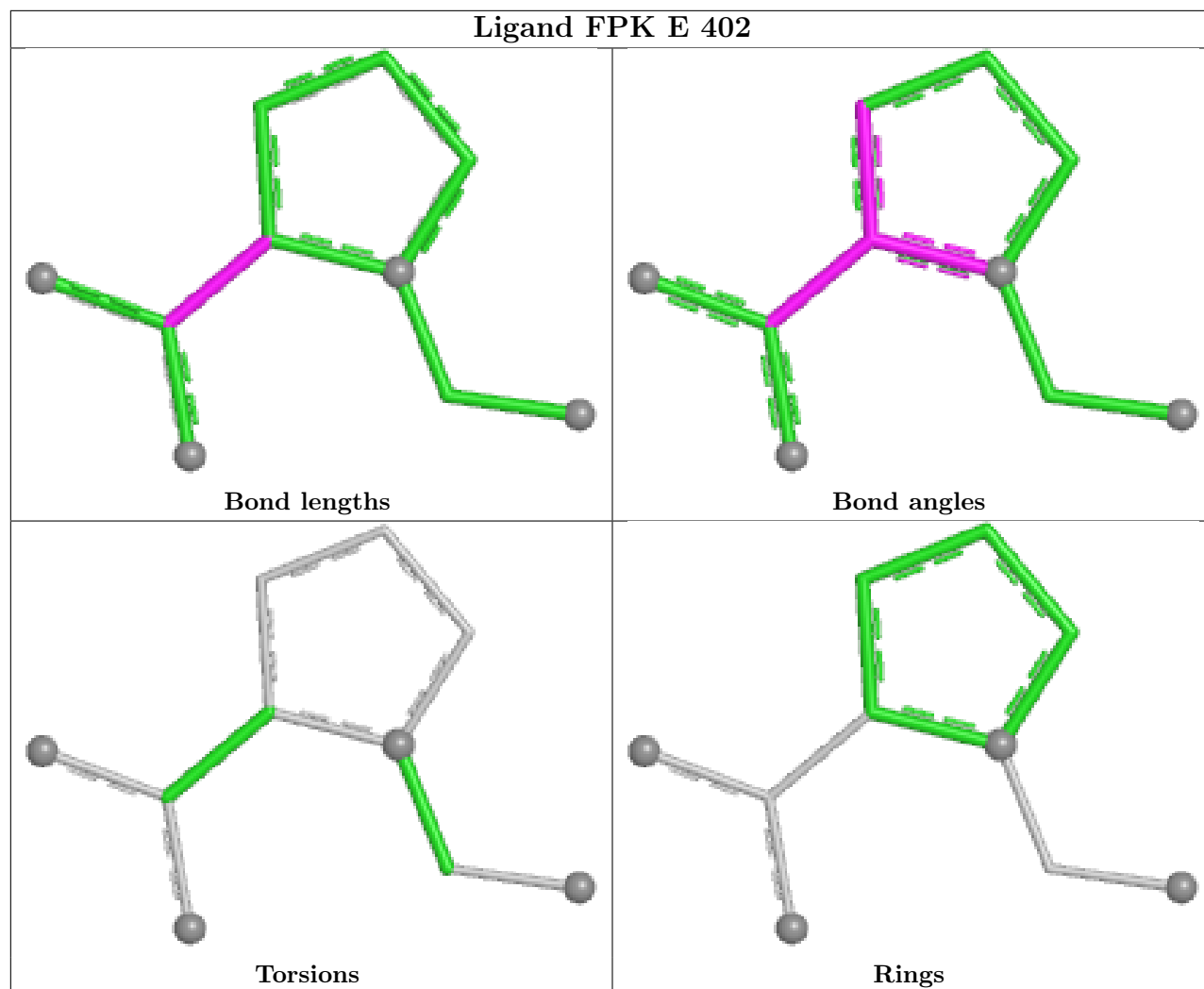
Ligand FPK D 402

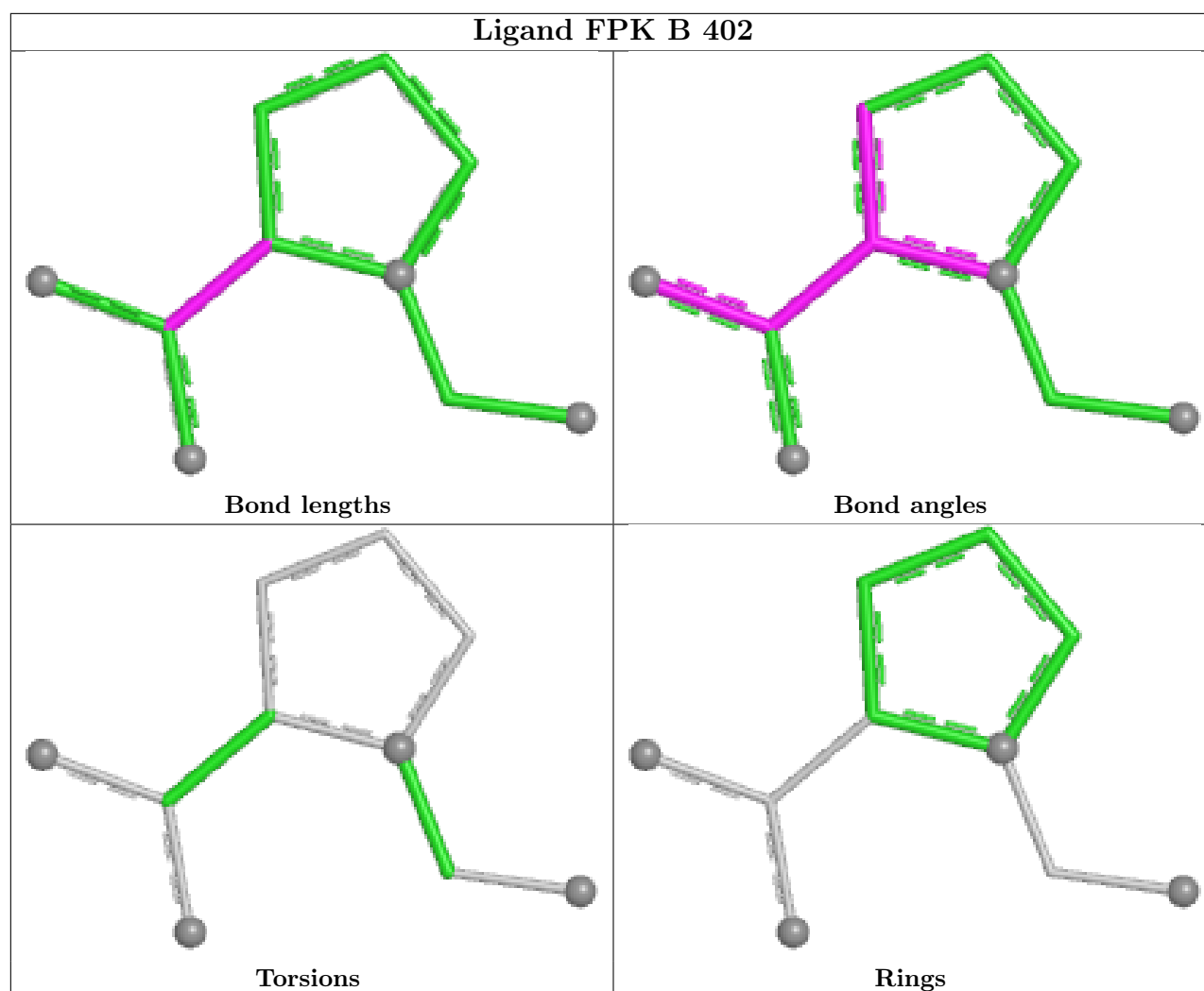






Ligand FPK E 402





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	278/316 (87%)	-0.13	8 (2%)	53	58	17, 30, 51, 73	4 (1%)
1	B	278/316 (87%)	-0.01	8 (2%)	53	58	17, 32, 54, 73	1 (0%)
1	C	276/316 (87%)	0.19	14 (5%)	33	35	19, 36, 60, 83	1 (0%)
1	D	276/316 (87%)	0.33	17 (6%)	26	28	18, 39, 67, 89	3 (1%)
1	E	276/316 (87%)	0.10	13 (4%)	36	38	17, 35, 63, 83	2 (0%)
All	All	1384/1580 (87%)	0.10	60 (4%)	40	42	17, 34, 62, 89	11 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-3	TYR	4.9
1	C	-2	PHE	4.6
1	E	-2	PHE	4.2
1	C	268	LEU	4.0
1	D	25	LEU	3.5
1	D	39	LEU	3.5
1	C	39	LEU	3.3
1	B	221	GLU	3.3
1	E	88	ASP	3.3
1	D	-2	PHE	3.3
1	C	38	ASP	3.2
1	B	270	SER	3.1
1	D	270	SER	3.1
1	C	273	ASP	3.0
1	B	38	ASP	2.9
1	C	143	VAL	2.9
1	D	143	VAL	2.9
1	B	272	ALA	2.9
1	D	28	HIS	2.9
1	A	-4	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	36	ASP	2.8
1	D	42	VAL	2.8
1	B	268	LEU	2.8
1	E	270	SER	2.7
1	E	268	LEU	2.6
1	C	78	ILE	2.6
1	B	39	LEU	2.6
1	D	78	ILE	2.6
1	D	269	GLN	2.6
1	A	272	ALA	2.6
1	B	143	VAL	2.6
1	E	143	VAL	2.6
1	E	271	MET	2.5
1	A	38	ASP	2.5
1	D	37	MET	2.5
1	C	37	MET	2.4
1	C	149	MET	2.4
1	B	37	MET	2.4
1	E	38	ASP	2.3
1	C	36	ASP	2.3
1	C	221	GLU	2.3
1	E	39	LEU	2.3
1	D	77	PHE	2.3
1	C	271	MET	2.3
1	E	272	ALA	2.3
1	E	23	GLY	2.3
1	E	0	SER	2.3
1	D	-1	GLN	2.3
1	A	-2	PHE	2.2
1	C	224	PRO	2.2
1	D	40	ALA	2.2
1	E	40	ALA	2.2
1	A	-5	ASN	2.2
1	A	270	SER	2.2
1	D	43	SER	2.2
1	A	271	MET	2.2
1	D	27	ALA	2.2
1	D	26	ALA	2.1
1	C	-1	GLN	2.1
1	E	-1	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

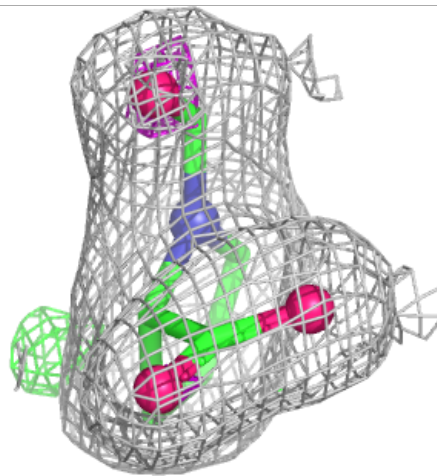
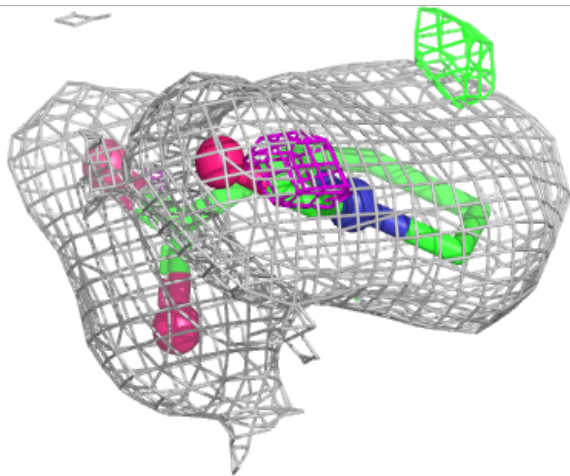
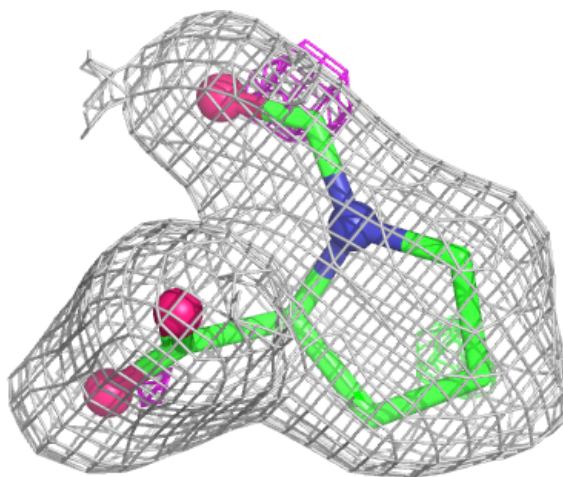
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	403	5/5	0.77	0.13	53,56,60,61	5
4	SO4	A	403	5/5	0.82	0.13	50,51,56,58	5
3	FPK	B	402	10/10	0.95	0.07	27,32,38,40	0
3	FPK	C	402	10/10	0.95	0.08	29,31,36,40	0
3	FPK	D	402	10/10	0.95	0.08	32,33,37,39	0
3	FPK	E	402	10/10	0.95	0.08	27,30,34,38	0
2	NAI	D	401	44/44	0.95	0.08	29,40,50,55	0
3	FPK	A	402	10/10	0.95	0.08	25,29,34,37	0
2	NAI	A	401	44/44	0.97	0.06	25,31,36,39	0
2	NAI	E	401	44/44	0.97	0.07	25,33,41,44	0
2	NAI	C	401	44/44	0.97	0.07	28,35,42,45	0
2	NAI	B	401	44/44	0.98	0.06	24,30,37,39	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.

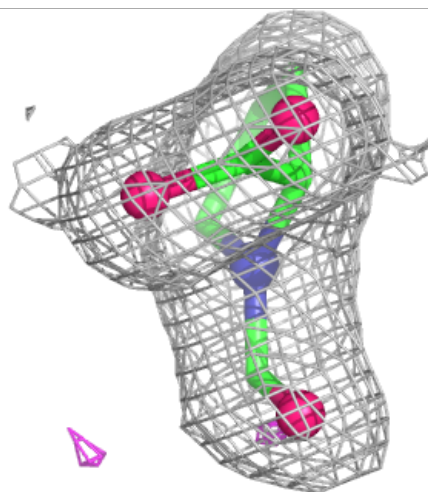
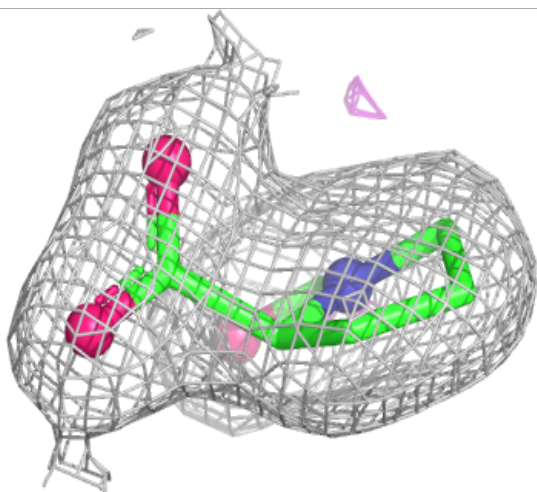
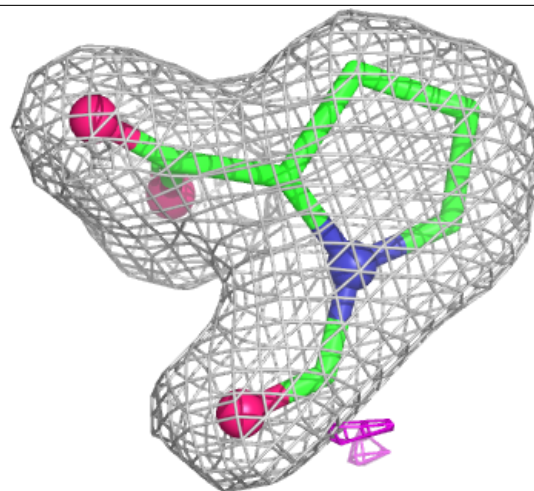
Electron density around FPK B 402:

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



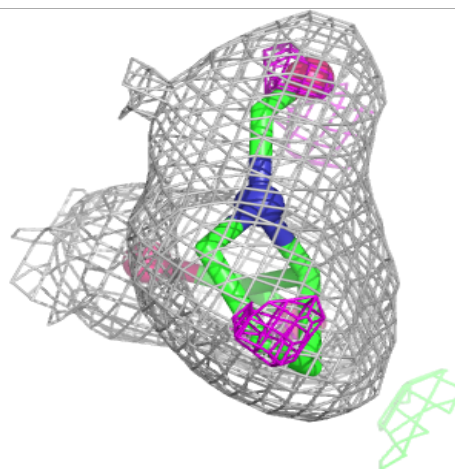
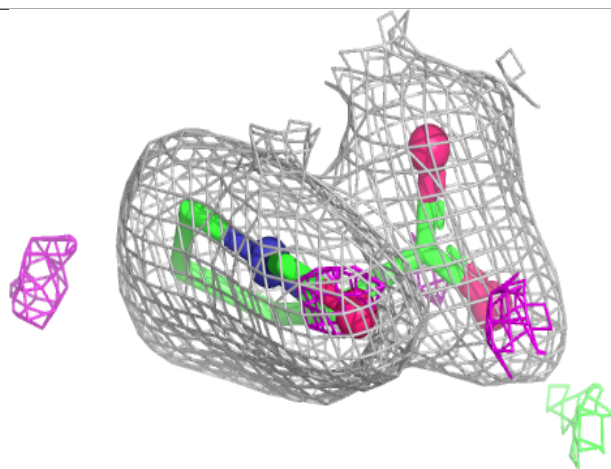
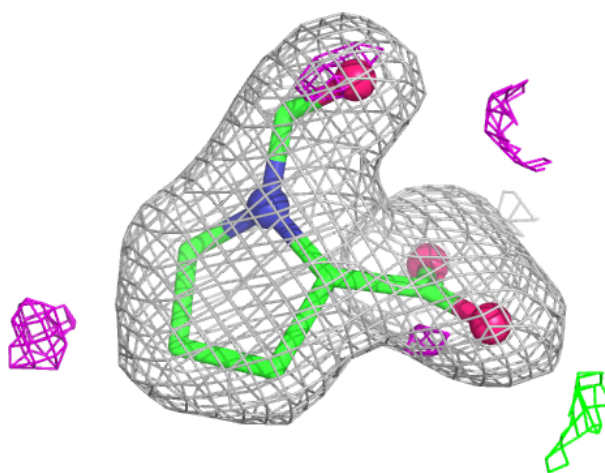
Electron density around FPK C 402:

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



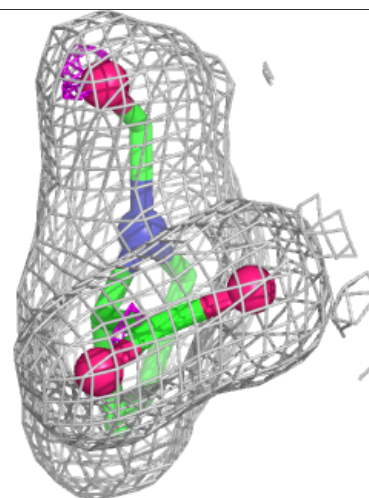
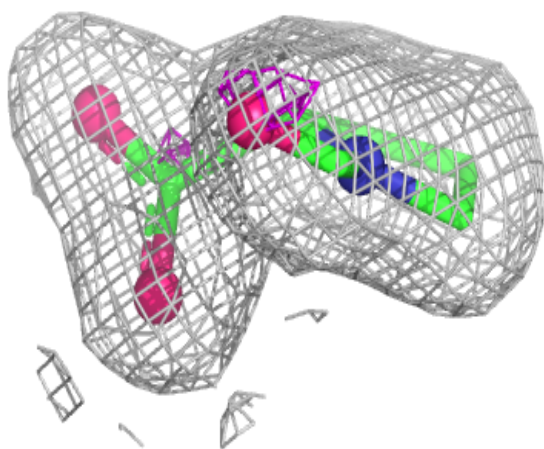
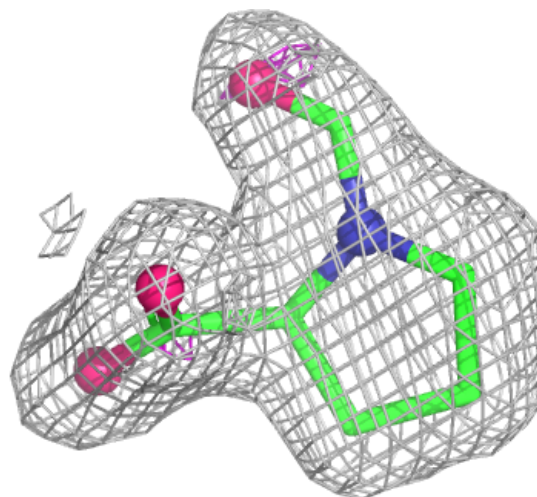
Electron density around FPK D 402:

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



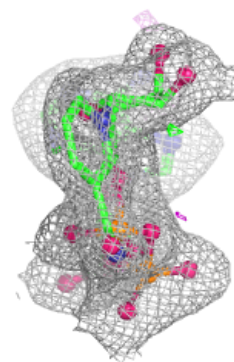
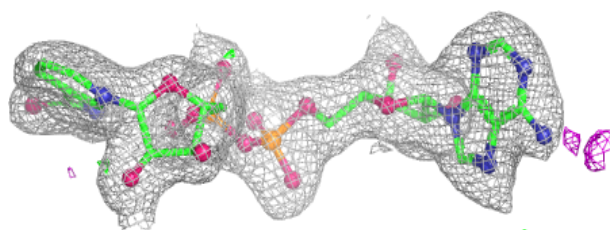
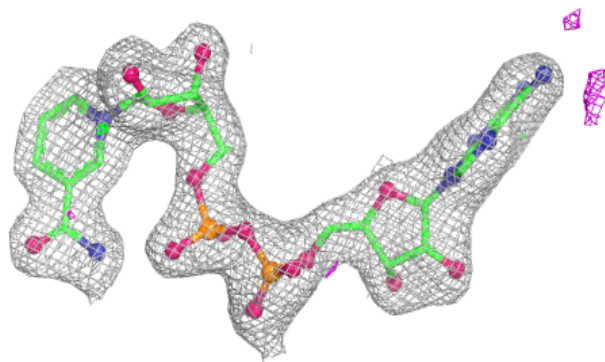
Electron density around FPK E 402:

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and green (positive)



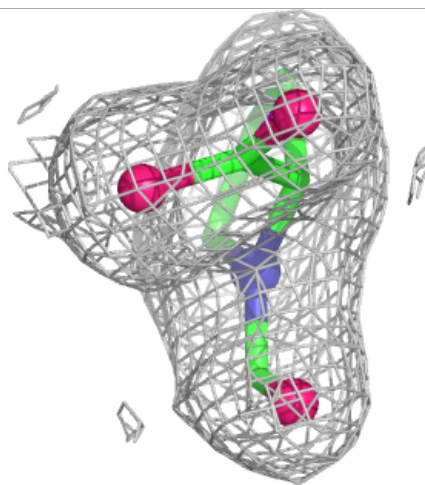
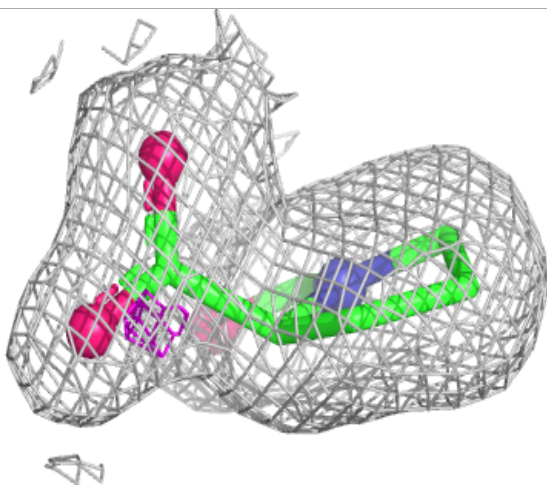
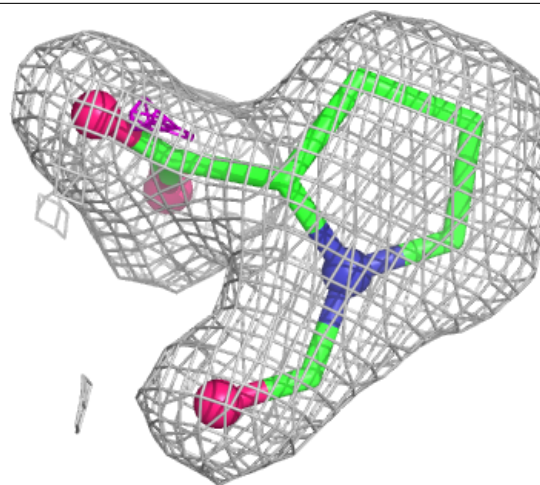
Electron density around NAI D 401:

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



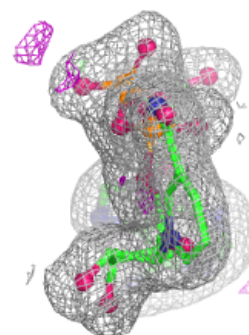
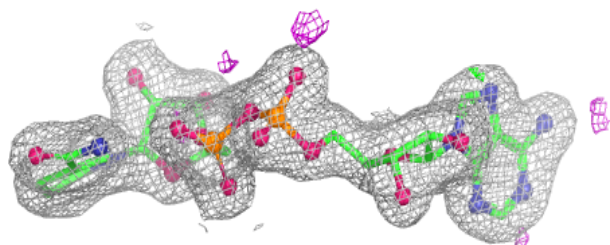
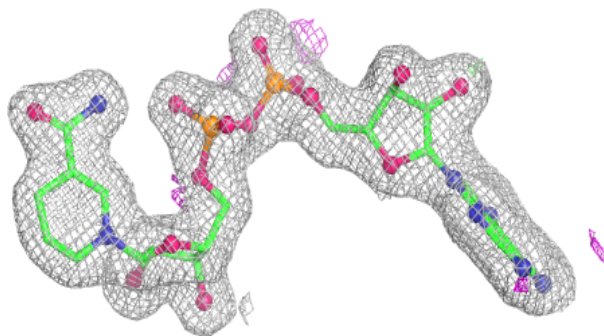
Electron density around FPK A 402:

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and green (positive)

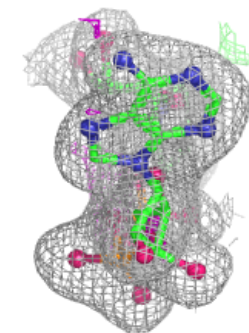
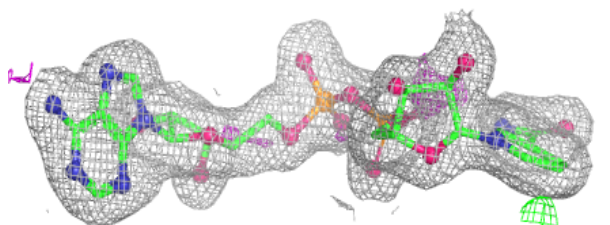
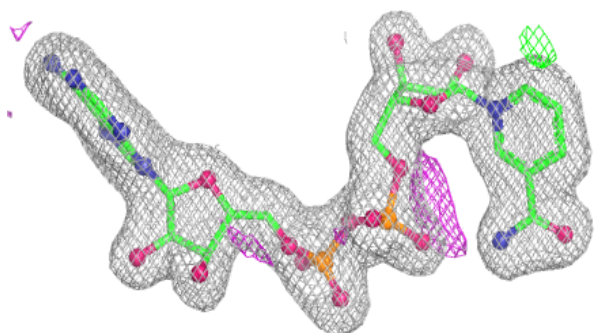


Electron density around NAI A 401:

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

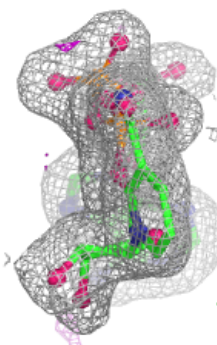
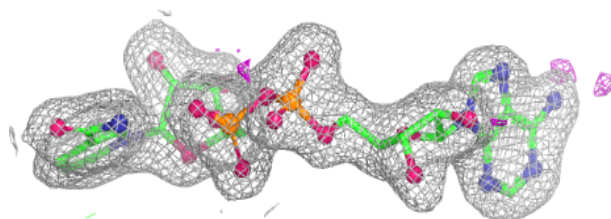
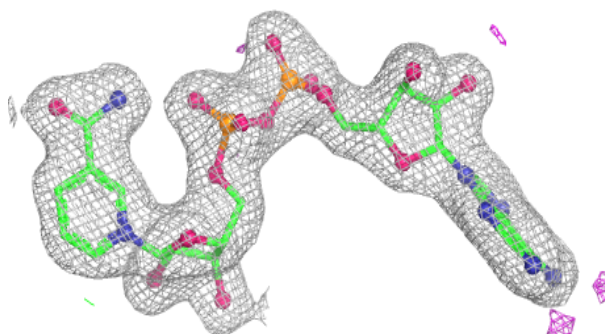
**Electron density around NAI E 401:**

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

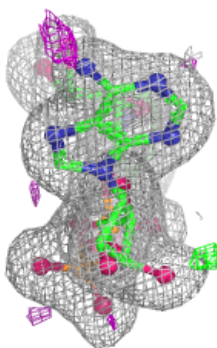
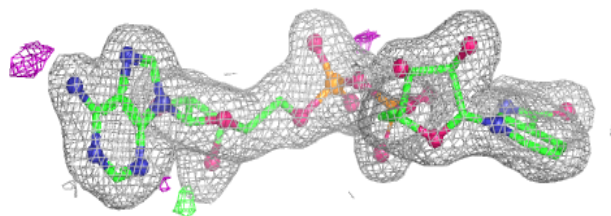
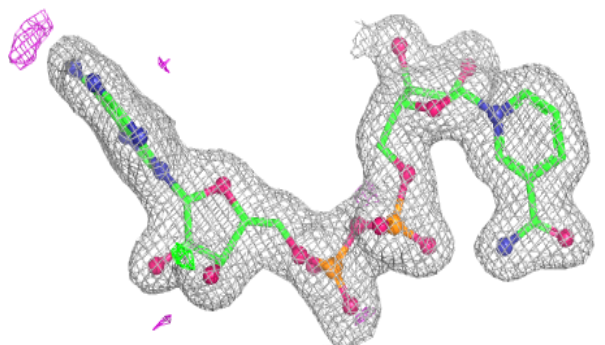


Electron density around NAI C 401:

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

**Electron density around NAI B 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.