



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2026 – 10:23 PM UTC

PDB ID : 8TDD / pdb_00008tdd
Title : Structure of PYCR1 complexed with NADH and 2-(furan-2-yl)acetic acid
Authors : Tanner, J.J.; Meeks, K.R.
Deposited on : 2023-07-02
Resolution : 1.91 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 : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.48.1

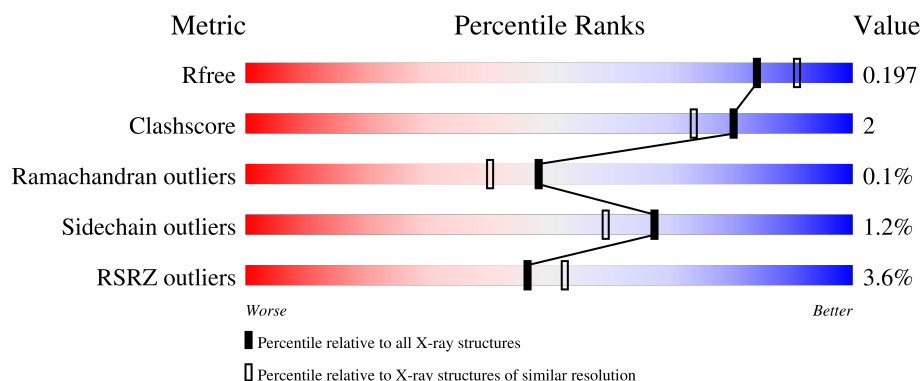
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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}	164625	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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% 83% 5% 12%
1	B	316	2% 84% 5% 11%
1	C	316	2% 82% 6% 12%
1	D	316	6% 82% 6% 11%
1	E	316	3% 82% 5% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11137 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	5	0
			2041	1286	359	383	13			
1	B	281	Total	C	N	O	S	0	5	0
			2055	1299	361	382	13			
1	C	278	Total	C	N	O	S	0	3	0
			2012	1269	356	373	14			
1	D	280	Total	C	N	O	S	0	3	0
			2029	1284	360	372	13			
1	E	278	Total	C	N	O	S	0	3	0
			2012	1269	356	373	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

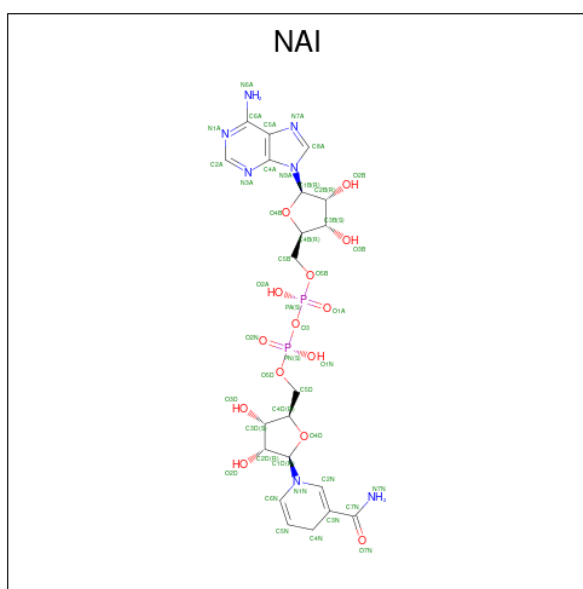
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	LEU	-	expression tag	UNP P32322
C	-3	TYR	-	expression tag	UNP P32322
C	-2	PHE	-	expression tag	UNP P32322
C	-1	GLN	-	expression tag	UNP P32322
C	0	SER	-	expression tag	UNP P32322
D	-21	MET	-	initiating methionine	UNP P32322
D	-20	HIS	-	expression tag	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

Continued on next page...

Continued from previous page...

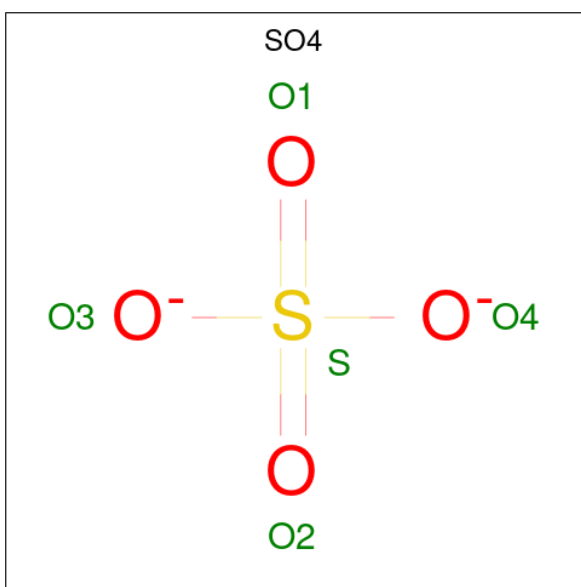
Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	GLU	-	expression tag	UNP P32322
E	-5	ASN	-	expression tag	UNP P32322
E	-4	LEU	-	expression tag	UNP P32322
E	-3	TYR	-	expression tag	UNP P32322
E	-2	PHE	-	expression tag	UNP P32322
E	-1	GLN	-	expression tag	UNP P32322
E	0	SER	-	expression tag	UNP P32322

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



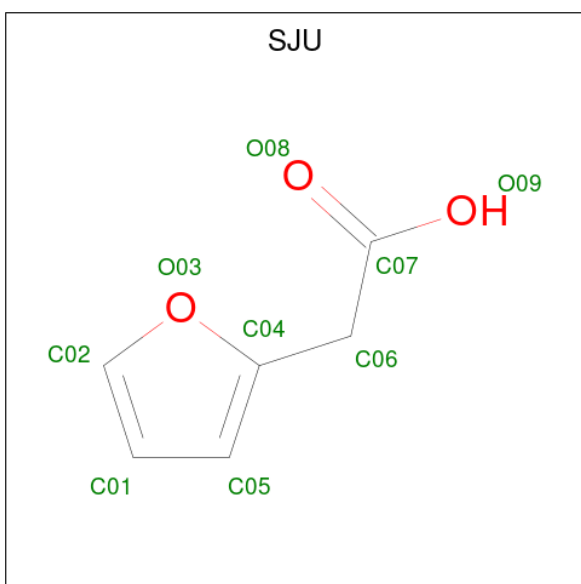
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 4 is (furan-2-yl)acetic acid (CCD ID: SJU) (formula: C₆H₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	1
			18	12	6		
4	C	1	Total	C	O	0	1
			18	12	6		

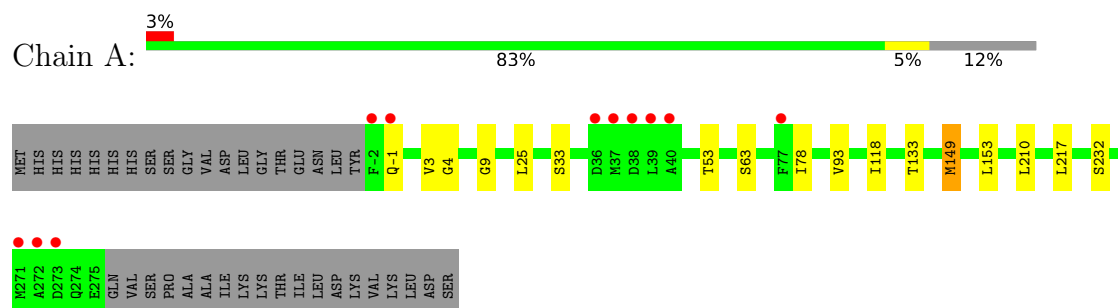
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	168	Total	O	0	0
			168	168		
5	B	158	Total	O	0	0
			158	158		
5	C	129	Total	O	0	0
			129	129		
5	D	119	Total	O	0	0
			119	119		
5	E	138	Total	O	0	0
			138	138		

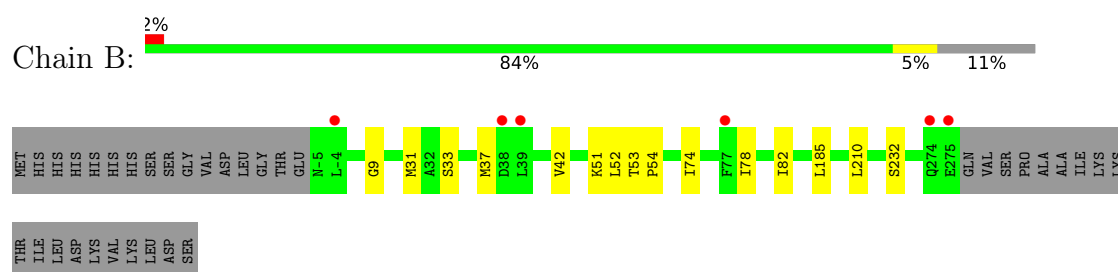
3 Residue-property plots [i](#)

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

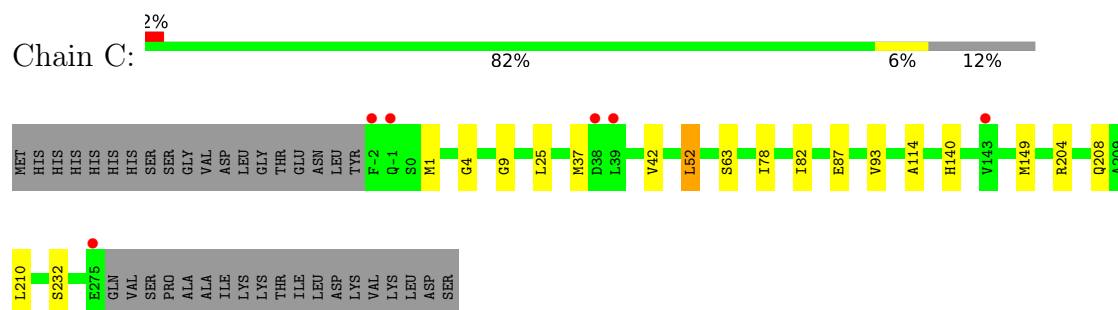
- Molecule 1: Pyrroline-5-carboxylate reductase 1, mitochondrial



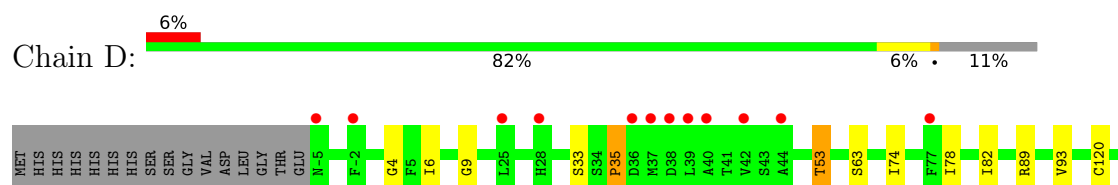
- Molecule 1: Pyrroline-5-carboxylate reductase 1, mitochondrial

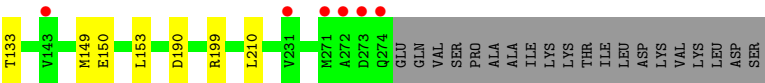


- Molecule 1: Pyrroline-5-carboxylate reductase 1, mitochondrial

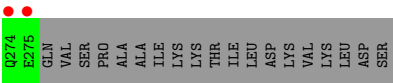
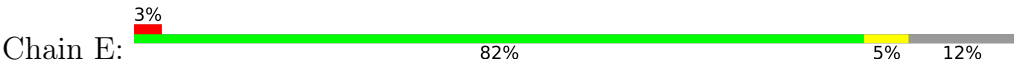


- Molecule 1: Pyrroline-5-carboxylate reductase 1, mitochondrial





● 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	111.09Å 180.47Å 88.10Å 90.00° 106.63° 90.00°	Depositor
Resolution (Å)	91.68 – 1.91 91.68 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.5 (91.68-1.91) 99.5 (91.68-1.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.20.1-4887	Depositor
R, R_{free}	0.167 , 0.197 0.167 , 0.197	Depositor DCC
R_{free} test set	6287 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11137	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, SJU, 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	0.32	0/2087	0.50	0/2830
1	B	0.31	0/2102	0.48	0/2853
1	C	0.28	0/2052	0.46	0/2785
1	D	0.27	0/2071	0.44	0/2813
1	E	0.30	0/2052	0.45	0/2784
All	All	0.30	0/10364	0.47	0/14065

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	2041	0	2074	12	0
1	B	2055	0	2078	11	0
1	C	2012	0	2029	10	0
1	D	2029	0	2036	13	0
1	E	2012	0	2035	9	0
2	A	44	0	27	1	0
2	B	44	0	27	1	0
2	C	44	0	27	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	44	0	27	2	0
2	E	44	0	27	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	B	18	0	0	0	0
4	C	18	0	0	0	0
5	A	168	0	0	0	0
5	B	158	0	0	0	0
5	C	129	0	0	0	0
5	D	119	0	0	0	0
5	E	138	0	0	0	0
All	All	11137	0	10387	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (51) 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:C:42:VAL:HG13	1:C:52:LEU:HD22	1.68	0.75
1:D:133:THR:HG21	1:D:153:LEU:HD13	1.73	0.71
1:A:210[A]:LEU:HD11	1:B:210[A]:LEU:HD13	1.72	0.71
1:A:210[B]:LEU:HD13	1:B:210[B]:LEU:HD11	1.72	0.69
1:D:63:SER:O	1:D:89:ARG:NH2	2.27	0.67
1:A:133:THR:HG21	1:A:153:LEU:HD13	1.76	0.67
1:C:210:LEU:HD13	1:D:210:LEU:HD11	1.78	0.65
1:E:133:THR:HG21	1:E:153:LEU:HD13	1.82	0.60
1:D:190:ASP:OD1	1:D:199[B]:ARG:NH2	2.34	0.55
1:D:93:VAL:HG21	1:D:149[A]:MET:HE1	1.89	0.54
1:D:78:ILE:O	1:D:82:ILE:HG13	2.09	0.53
1:E:3:VAL:HG21	1:E:25:LEU:HD11	1.91	0.52
1:D:6[B]:ILE:HG21	1:D:78:ILE:HG21	1.91	0.51
1:C:1:MET:HE2	1:C:25:LEU:HD21	1.94	0.50
1:D:6[A]:ILE:HG21	1:D:78:ILE:HG21	1.94	0.49
1:A:33:SER:HA	1:A:53:THR:O	2.14	0.48
1:B:74:ILE:HG22	1:B:78:ILE:HG12	1.97	0.47
1:B:9:GLY:HA3	2:B:401:NAI:O5B	2.16	0.46
1:E:78:ILE:O	1:E:82:ILE:HG13	2.16	0.46
1:A:149[A]:MET:HB3	1:A:149[A]:MET:HE3	1.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ILE:O	1:C:82:ILE:HG13	2.16	0.46
1:B:37:MET:HE2	1:B:54:PRO:HD3	1.97	0.45
1:A:217:LEU:HD23	1:B:185:LEU:HD13	1.98	0.45
1:E:93:VAL:HG21	1:E:149[B]:MET:HE2	1.98	0.45
1:C:37:MET:HA	1:C:37:MET:HE2	1.99	0.45
1:C:93:VAL:HG21	1:C:149[B]:MET:HE2	1.98	0.45
1:E:8:ALA:HB3	1:E:34:SER:HB2	1.99	0.45
1:A:4:GLY:HA3	1:A:63:SER:OG	2.17	0.44
1:A:9:GLY:HA3	2:A:401:NAI:O5B	2.18	0.44
1:A:118:ILE:HG21	1:A:149[A]:MET:HE2	2.00	0.43
1:E:33:SER:HA	1:E:53:THR:O	2.19	0.43
1:B:33:SER:HA	1:B:53:THR:O	2.19	0.42
1:C:9:GLY:HA3	2:C:401:NAI:O5B	2.19	0.42
1:B:37:MET:HE1	1:B:52:LEU:HB3	2.02	0.42
1:A:78:ILE:HD13	1:A:78:ILE:HA	1.83	0.41
1:D:4:GLY:HA3	1:D:63:SER:OG	2.20	0.41
1:B:42:VAL:HG13	1:B:52:LEU:HD13	2.02	0.41
1:D:33:SER:HA	1:D:53:THR:O	2.20	0.41
1:B:31:MET:HA	1:B:51:LYS:O	2.20	0.41
1:B:78:ILE:O	1:B:82:ILE:HG13	2.21	0.41
1:D:74:ILE:HG22	1:D:78:ILE:HG12	2.03	0.41
1:C:114:ALA:HA	1:C:140:HIS:CD2	2.55	0.41
1:E:37:MET:HE1	1:E:52:LEU:HB3	2.03	0.41
1:D:35:PRO:HD3	2:D:401:NAI:C4A	2.51	0.41
1:E:118:ILE:HD12	1:E:149[B]:MET:HG3	2.03	0.41
1:E:241:ALA:O	1:E:244:VAL:HG22	2.21	0.41
1:A:93:VAL:HG21	1:A:149[B]:MET:HE2	2.03	0.41
1:C:4:GLY:HA3	1:C:63:SER:OG	2.21	0.40
1:D:9:GLY:HA3	2:D:401:NAI:O5B	2.21	0.40
1:A:3:VAL:HG21	1:A:25:LEU:HD11	2.02	0.40
1:C:204[A]:ARG:NH1	1:C:208:GLN:HB2	2.36	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	281/316 (89%)	276 (98%)	5 (2%)	0	100	100
1	B	284/316 (90%)	281 (99%)	3 (1%)	0	100	100
1	C	279/316 (88%)	275 (99%)	4 (1%)	0	100	100
1	D	281/316 (89%)	275 (98%)	5 (2%)	1 (0%)	30	19
1	E	279/316 (88%)	274 (98%)	5 (2%)	0	100	100
All	All	1404/1580 (89%)	1381 (98%)	22 (2%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	35	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	213/251 (85%)	209 (98%)	4 (2%)	52	39
1	B	211/251 (84%)	210 (100%)	1 (0%)	86	85
1	C	205/251 (82%)	202 (98%)	3 (2%)	60	49
1	D	204/251 (81%)	201 (98%)	3 (2%)	60	49
1	E	206/251 (82%)	203 (98%)	3 (2%)	60	49
All	All	1039/1255 (83%)	1025 (99%)	14 (1%)	67	55

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	GLN
1	A	149[A]	MET
1	A	149[B]	MET
1	A	232	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	232	SER
1	C	52	LEU
1	C	87	GLU
1	C	232	SER
1	D	53	THR
1	D	120	CYS
1	D	150	GLU
1	E	149[A]	MET
1	E	149[B]	MET
1	E	210	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	B	61	GLN
1	B	140	HIS
1	C	28	HIS
1	C	140	HIS
1	C	219	HIS
1	C	226	GLN
1	D	61	GLN
1	D	226	GLN
1	D	230	ASN
1	E	222	GLN
1	E	226	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

13 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	SO4	D	402	-	4,4,4	0.27	0	6,6,6	0.17	0
4	SJU	C	402[B]	-	6,9,9	3.51	1 (16%)	7,11,11	1.49	3 (42%)
2	NAI	C	401	-	43,48,48	1.43	9 (20%)	50,73,73	1.77	12 (24%)
3	SO4	C	403	-	4,4,4	0.28	0	6,6,6	0.18	0
2	NAI	D	401	-	43,48,48	1.50	7 (16%)	50,73,73	1.84	15 (30%)
4	SJU	B	402[B]	-	6,9,9	2.94	2 (33%)	7,11,11	1.35	1 (14%)
2	NAI	E	401	-	43,48,48	1.44	8 (18%)	50,73,73	1.78	12 (24%)
4	SJU	C	402[A]	-	6,9,9	3.20	1 (16%)	7,11,11	1.45	2 (28%)
3	SO4	B	403	-	4,4,4	0.31	0	6,6,6	0.16	0
2	NAI	B	401	-	43,48,48	1.38	7 (16%)	50,73,73	1.80	12 (24%)
3	SO4	A	402	-	4,4,4	0.24	0	6,6,6	0.17	0
4	SJU	B	402[A]	-	6,9,9	2.93	2 (33%)	7,11,11	1.33	1 (14%)
2	NAI	A	401	-	43,48,48	1.39	6 (13%)	50,73,73	1.84	11 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SJU	C	402[B]	-	-	0/2/4/4	0/1/1/1
2	NAI	C	401	-	-	4/25/72/72	0/5/5/5
2	NAI	D	401	-	-	7/25/72/72	0/5/5/5
4	SJU	B	402[B]	-	-	0/2/4/4	0/1/1/1
2	NAI	E	401	-	-	5/25/72/72	0/5/5/5
4	SJU	C	402[A]	-	-	0/2/4/4	0/1/1/1
2	NAI	B	401	-	-	3/25/72/72	0/5/5/5
4	SJU	B	402[A]	-	-	0/2/4/4	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	A	401	-	-	4/25/72/72	0/5/5/5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402[B]	SJU	C06-C04	-7.93	1.45	1.51
4	C	402[A]	SJU	C06-C04	-7.08	1.46	1.51
4	B	402[A]	SJU	C06-C04	-6.55	1.46	1.51
4	B	402[B]	SJU	C06-C04	-6.50	1.46	1.51
2	A	401	NAI	PA-O5B	3.79	1.74	1.59
2	E	401	NAI	PN-O5D	3.76	1.74	1.59
2	C	401	NAI	PA-O5B	3.59	1.73	1.59
2	D	401	NAI	PA-O5B	3.58	1.73	1.59
2	D	401	NAI	PN-O3	3.53	1.63	1.59
2	B	401	NAI	PN-O5D	3.52	1.73	1.59
2	E	401	NAI	PA-O5B	3.52	1.73	1.59
2	B	401	NAI	PA-O5B	3.43	1.72	1.59
2	D	401	NAI	PN-O5D	3.25	1.72	1.59
2	C	401	NAI	PN-O5D	3.17	1.71	1.59
2	A	401	NAI	PN-O3	2.77	1.62	1.59
2	A	401	NAI	PN-O5D	2.76	1.70	1.59
2	D	401	NAI	PA-O3	2.67	1.62	1.59
2	B	401	NAI	C3B-C4B	2.60	1.59	1.53
2	C	401	NAI	C4A-N3A	2.46	1.39	1.35
2	E	401	NAI	C2A-N1A	2.45	1.38	1.33
2	D	401	NAI	C2A-N3A	2.40	1.35	1.32
2	C	401	NAI	C6N-N1N	2.40	1.43	1.37
2	C	401	NAI	C2A-N3A	2.40	1.35	1.32
2	E	401	NAI	O5D-C5D	-2.34	1.35	1.44
2	B	401	NAI	C2A-N3A	2.27	1.35	1.32
2	A	401	NAI	C7N-N7N	2.24	1.39	1.33
2	D	401	NAI	C2A-N1A	2.20	1.37	1.33
2	A	401	NAI	C2A-N3A	2.19	1.35	1.32
4	B	402[B]	SJU	C06-C07	2.18	1.55	1.51
2	C	401	NAI	C7N-N7N	2.17	1.39	1.33
2	C	401	NAI	C2A-N1A	2.16	1.37	1.33
2	E	401	NAI	PN-O3	2.15	1.61	1.59
2	C	401	NAI	C3B-C4B	2.15	1.58	1.53
2	E	401	NAI	C3B-C4B	2.14	1.58	1.53
2	A	401	NAI	C3D-C4D	2.12	1.58	1.53
2	E	401	NAI	C1B-N9A	-2.12	1.44	1.49
2	B	401	NAI	C2A-N1A	2.07	1.37	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NAI	PN-O3	2.06	1.61	1.59
2	D	401	NAI	C4A-N3A	2.06	1.38	1.35
2	B	401	NAI	C6N-N1N	2.04	1.42	1.37
2	B	401	NAI	PA-O3	2.03	1.61	1.59
2	E	401	NAI	C2A-N3A	2.03	1.35	1.32
4	B	402[A]	SJU	C06-C07	2.01	1.55	1.51

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAI	C4B-O4B-C1B	-5.81	104.60	109.92
2	A	401	NAI	C4B-O4B-C1B	-5.77	104.64	109.92
2	E	401	NAI	C4B-O4B-C1B	-5.77	104.64	109.92
2	C	401	NAI	C4B-O4B-C1B	-5.71	104.70	109.92
2	B	401	NAI	C4B-O4B-C1B	-5.60	104.80	109.92
2	A	401	NAI	O2A-PA-O3	4.80	120.25	107.27
2	B	401	NAI	O2A-PA-O3	4.23	118.71	107.27
2	B	401	NAI	O3-PA-O1A	-4.13	98.29	110.70
2	D	401	NAI	O2A-PA-O3	4.03	118.18	107.27
2	E	401	NAI	O2A-PA-O3	3.98	118.04	107.27
2	C	401	NAI	O2A-PA-O3	3.93	117.90	107.27
2	A	401	NAI	O1N-PN-O3	3.91	117.83	107.27
2	A	401	NAI	O3-PA-O1A	-3.90	98.96	110.70
2	E	401	NAI	O3-PA-O1A	-3.75	99.42	110.70
2	C	401	NAI	O3-PA-O1A	-3.71	99.53	110.70
2	B	401	NAI	O1N-PN-O3	3.62	117.06	107.27
2	D	401	NAI	O1N-PN-O3	3.55	116.88	107.27
2	D	401	NAI	O3-PA-O1A	-3.53	100.10	110.70
2	C	401	NAI	O1N-PN-O3	3.43	116.54	107.27
2	E	401	NAI	O2A-PA-O1A	3.15	127.12	112.44
2	B	401	NAI	O2A-PA-O1A	3.13	127.01	112.44
2	D	401	NAI	O2A-PA-O1A	3.12	126.97	112.44
2	E	401	NAI	O1N-PN-O2N	3.09	126.81	112.44
2	A	401	NAI	O2A-PA-O1A	3.09	126.80	112.44
2	C	401	NAI	O2A-PA-O1A	3.07	126.75	112.44
2	D	401	NAI	O1N-PN-O2N	3.02	126.48	112.44
2	E	401	NAI	O1N-PN-O3	3.00	115.38	107.27
2	C	401	NAI	O1N-PN-O2N	2.85	125.71	112.44
2	A	401	NAI	O1N-PN-O2N	2.83	125.61	112.44
2	B	401	NAI	O1N-PN-O2N	2.81	125.52	112.44
2	D	401	NAI	O5D-PN-O2N	-2.66	98.40	108.94
4	C	402[B]	SJU	O08-C07-C06	-2.57	115.18	122.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAI	O5D-PN-O2N	-2.54	98.88	108.94
4	C	402[A]	SJU	O08-C07-C06	-2.53	115.30	122.94
2	B	401	NAI	C1B-N9A-C4A	-2.51	122.24	126.64
2	D	401	NAI	O7N-C7N-N7N	-2.46	117.37	122.89
2	E	401	NAI	PA-O5B-C5B	-2.39	107.67	121.35
2	D	401	NAI	PA-O5B-C5B	-2.26	108.39	121.35
2	E	401	NAI	O5D-PN-O2N	-2.26	99.98	108.94
2	B	401	NAI	PA-O5B-C5B	-2.26	108.43	121.35
2	C	401	NAI	PA-O5B-C5B	-2.25	108.47	121.35
2	D	401	NAI	O3-PN-O2N	-2.24	103.96	110.70
2	A	401	NAI	C1B-N9A-C4A	-2.22	122.73	126.64
2	C	401	NAI	C5B-C4B-C3B	-2.21	107.25	115.21
2	B	401	NAI	O7N-C7N-N7N	-2.21	117.94	122.89
2	D	401	NAI	C1B-N9A-C4A	-2.21	122.77	126.64
2	D	401	NAI	C5B-C4B-C3B	-2.19	107.31	115.21
2	E	401	NAI	C5B-C4B-C3B	-2.18	107.36	115.21
2	C	401	NAI	PN-O5D-C5D	-2.17	108.89	121.35
2	A	401	NAI	C5B-C4B-C3B	-2.17	107.39	115.21
2	B	401	NAI	C5B-C4B-C3B	-2.15	107.49	115.21
4	B	402[B]	SJU	O08-C07-C06	-2.14	116.48	122.94
2	C	401	NAI	C4A-C5A-N7A	2.14	111.59	109.34
2	E	401	NAI	C1B-N9A-C4A	-2.13	122.91	126.64
2	B	401	NAI	O5D-PN-O2N	-2.12	100.52	108.94
2	A	401	NAI	O5B-PA-O1A	-2.12	100.53	108.94
2	D	401	NAI	O5B-PA-O1A	-2.08	100.68	108.94
2	E	401	NAI	O7N-C7N-N7N	-2.08	118.24	122.89
4	B	402[A]	SJU	O08-C07-C06	-2.07	116.69	122.94
2	A	401	NAI	C3N-C2N-N1N	-2.07	120.17	123.20
2	D	401	NAI	C3N-C2N-N1N	-2.06	120.19	123.20
4	C	402[B]	SJU	O09-C07-O08	2.05	128.61	123.33
4	C	402[A]	SJU	C05-C01-C02	-2.05	105.62	112.92
2	A	401	NAI	PA-O5B-C5B	-2.04	109.65	121.35
4	C	402[B]	SJU	C05-C01-C02	-2.04	105.65	112.92
2	C	401	NAI	O3-PN-O2N	-2.04	104.56	110.70
2	B	401	NAI	C3N-C2N-N1N	-2.01	120.25	123.20
2	E	401	NAI	O3-PN-O2N	-2.01	104.67	110.70
2	D	401	NAI	PN-O5D-C5D	-2.00	109.89	121.35

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	NAI	C2N-C3N-C7N-N7N
2	D	401	NAI	C5D-O5D-PN-O3
2	D	401	NAI	C5D-O5D-PN-O2N
2	E	401	NAI	C2N-C3N-C7N-N7N
2	D	401	NAI	O4D-C4D-C5D-O5D
2	C	401	NAI	O4D-C4D-C5D-O5D
2	D	401	NAI	PN-O3-PA-O1A
2	D	401	NAI	PN-O3-PA-O2A
2	C	401	NAI	O4D-C1D-N1N-C6N
2	B	401	NAI	O4D-C1D-N1N-C6N
2	D	401	NAI	O4D-C1D-N1N-C6N
2	D	401	NAI	C3D-C4D-C5D-O5D
2	E	401	NAI	O4D-C1D-N1N-C6N
2	A	401	NAI	O4D-C1D-N1N-C6N
2	A	401	NAI	PN-O3-PA-O2A
2	E	401	NAI	C2D-C1D-N1N-C6N
2	B	401	NAI	C2D-C1D-N1N-C6N
2	E	401	NAI	O4D-C4D-C5D-O5D
2	B	401	NAI	PN-O3-PA-O2A
2	A	401	NAI	O4B-C4B-C5B-O5B
2	A	401	NAI	O4D-C4D-C5D-O5D
2	C	401	NAI	PN-O3-PA-O2A
2	E	401	NAI	PN-O3-PA-O2A

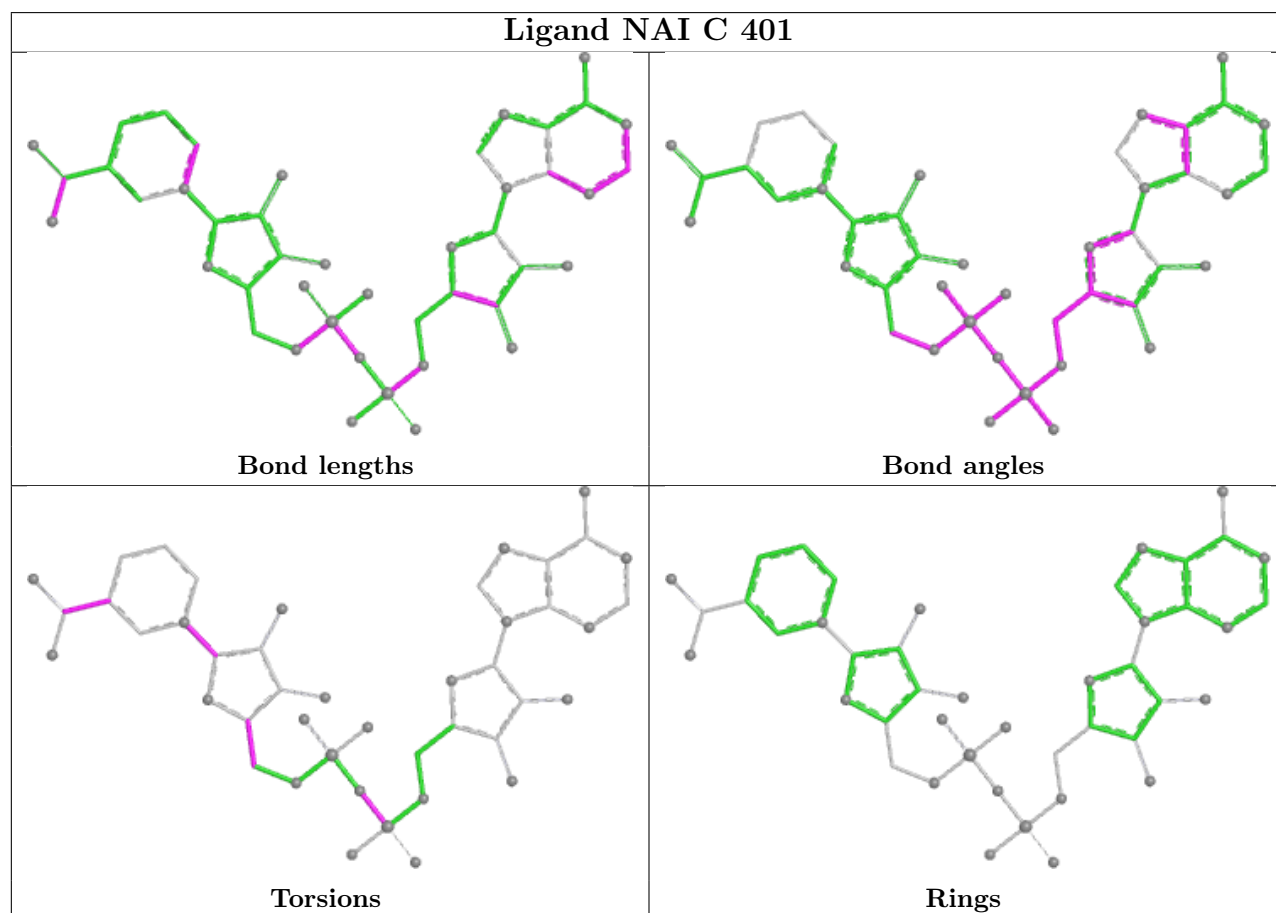
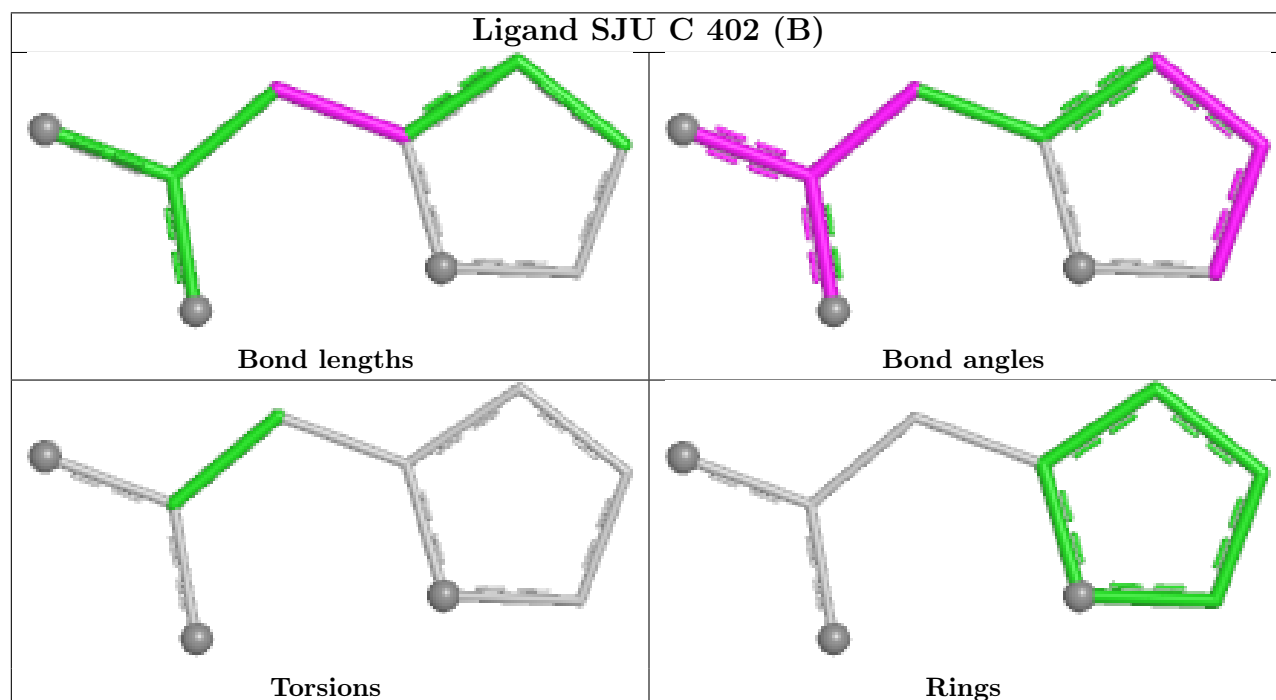
There are no ring outliers.

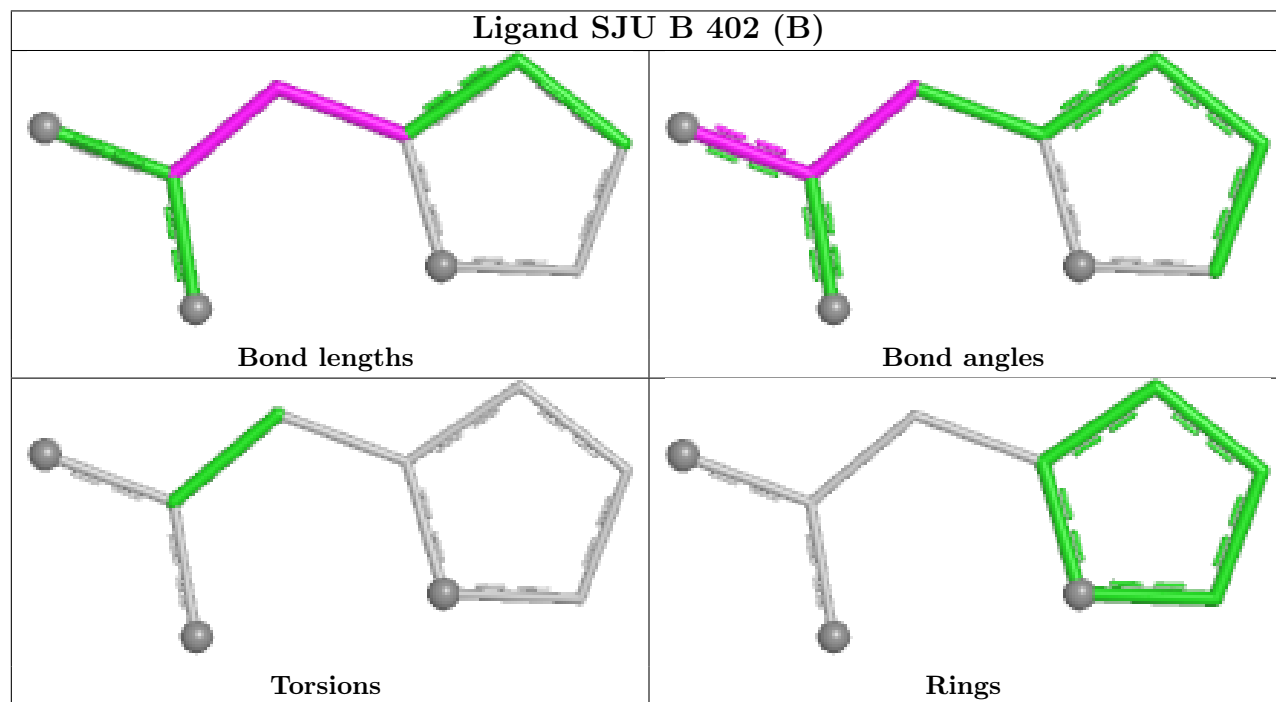
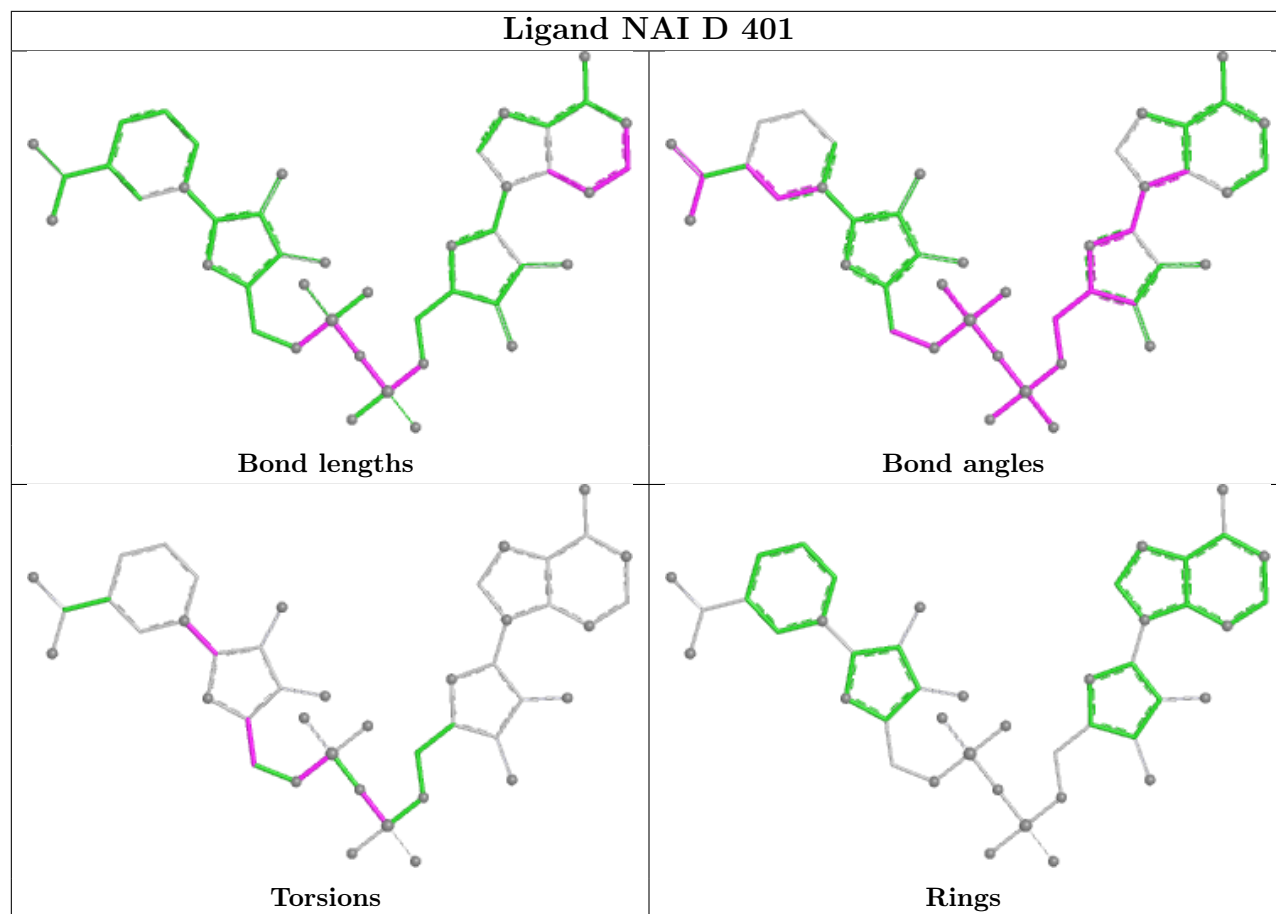
4 monomers are involved in 5 short contacts:

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

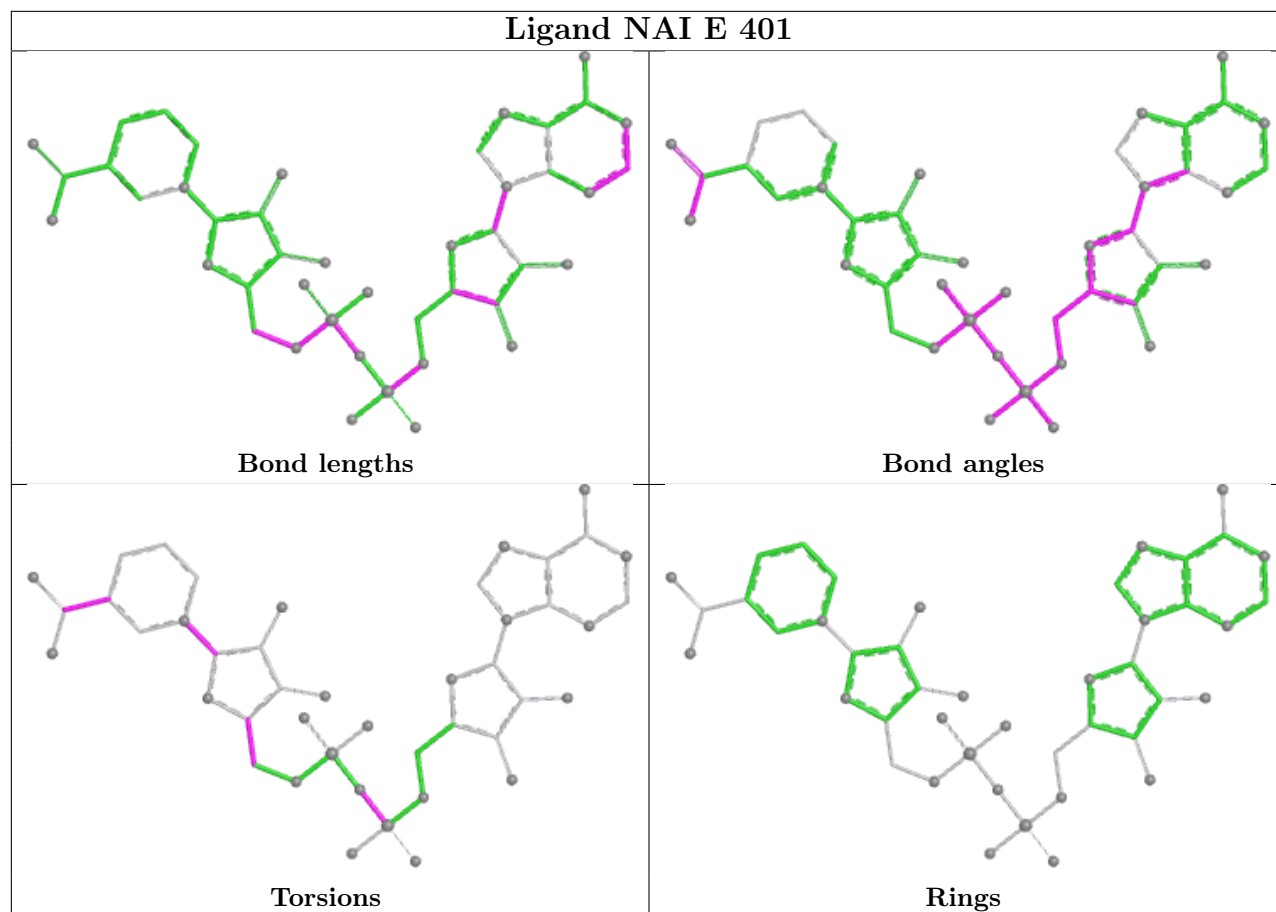
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

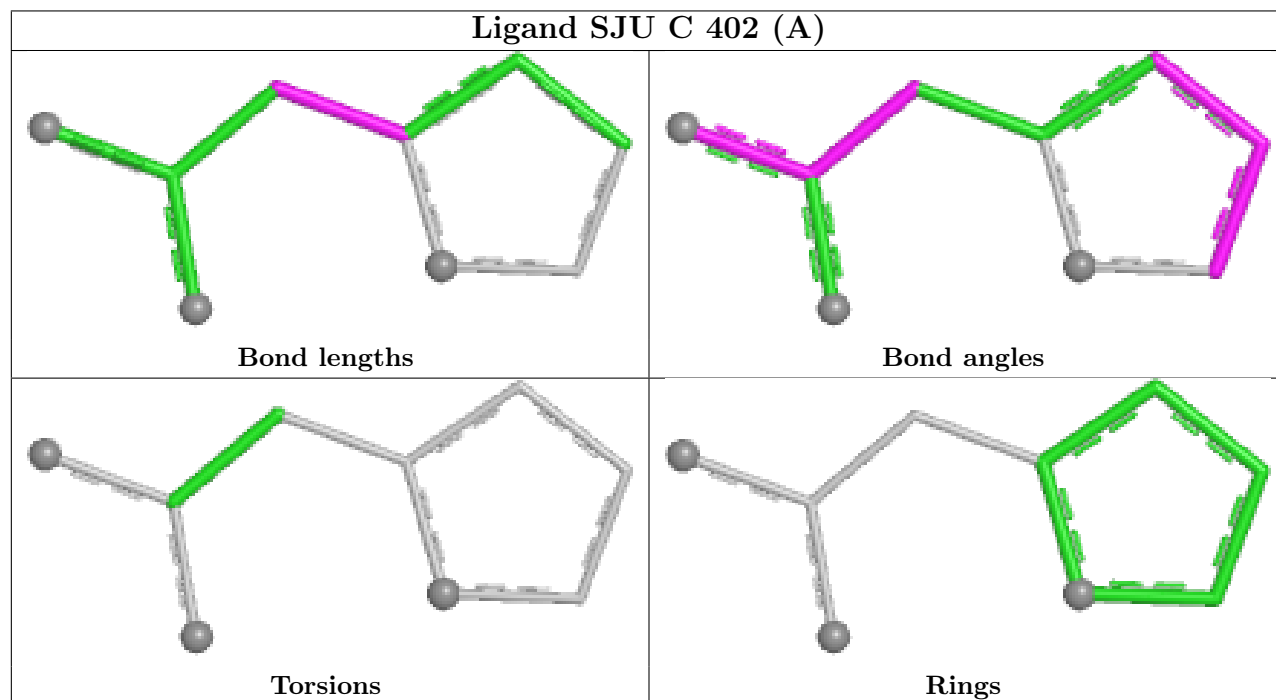


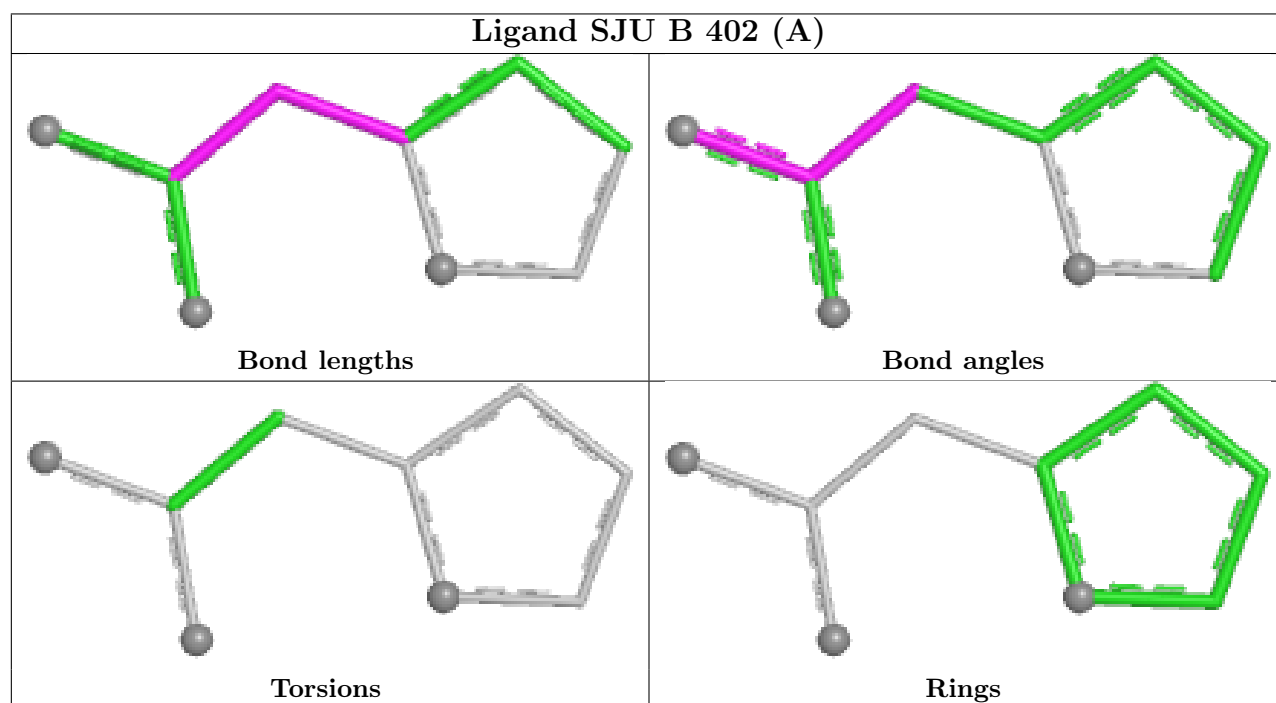
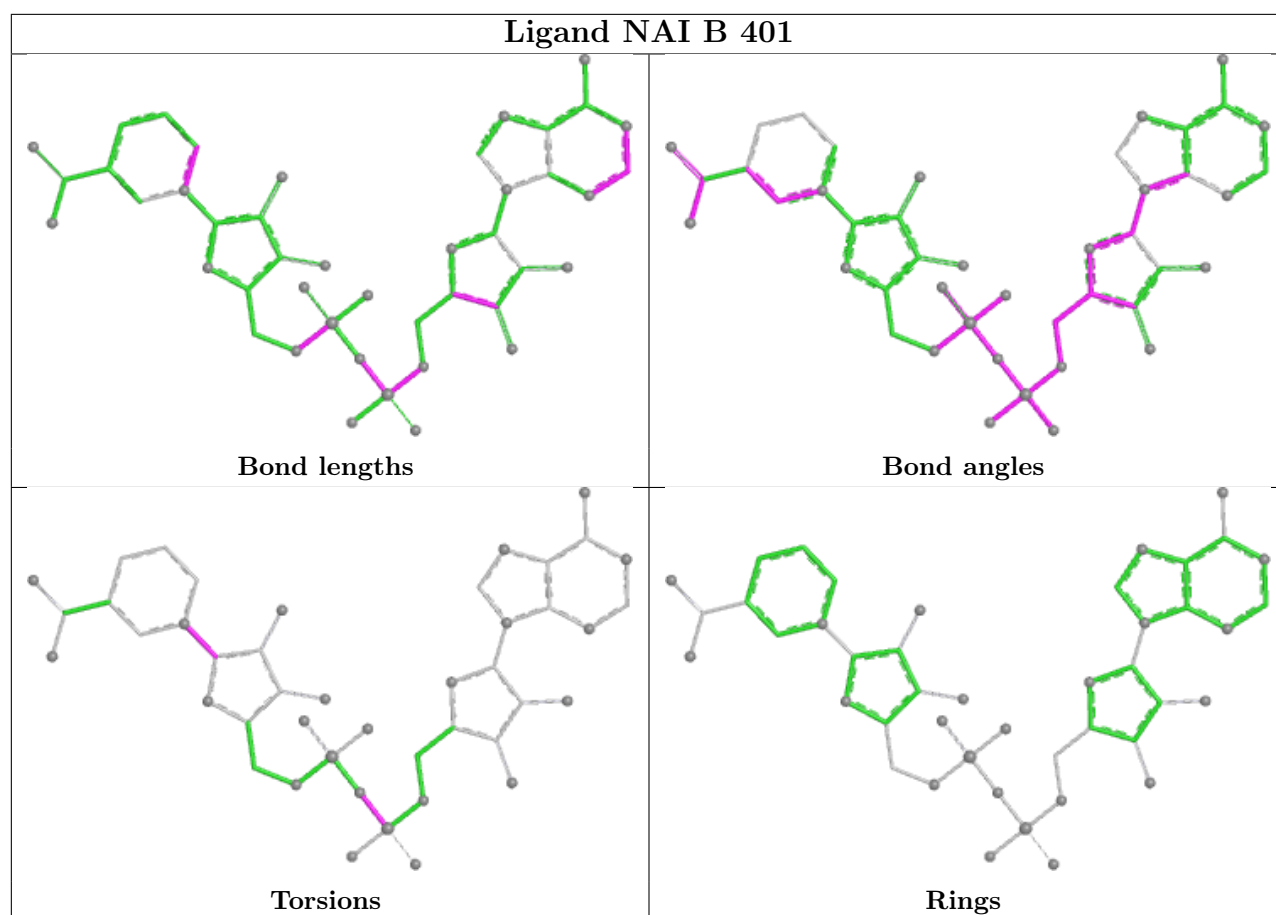


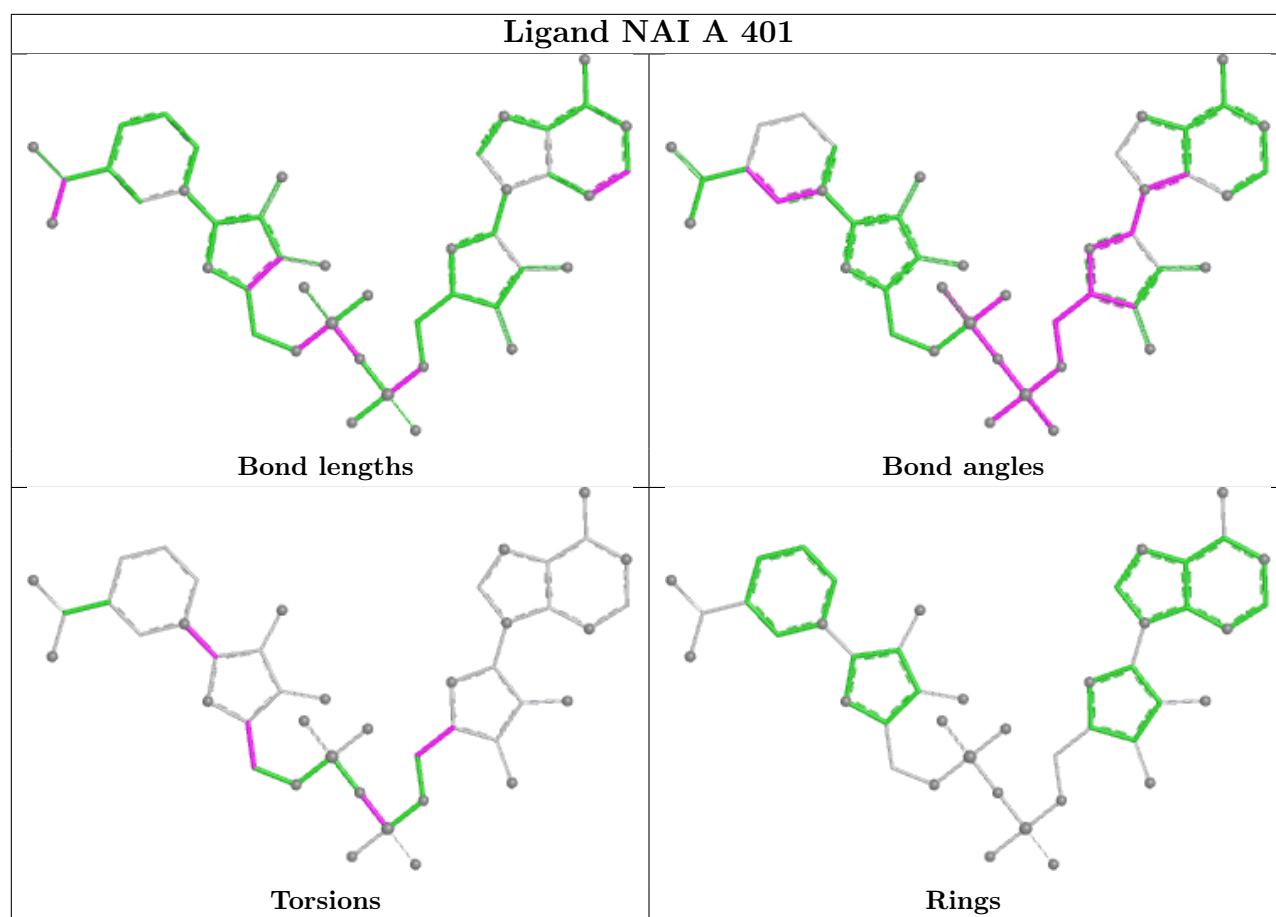
Ligand NAI E 401



Ligand SJU C 402 (A)







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%)	-0.21	11 (3%) 43 48	14, 28, 53, 88	5 (1%)
1	B	281/316 (88%)	-0.16	6 (2%) 63 69	14, 30, 53, 77	5 (1%)
1	C	278/316 (87%)	-0.06	6 (2%) 62 67	16, 34, 58, 81	3 (1%)
1	D	280/316 (88%)	0.23	18 (6%) 27 32	16, 38, 70, 87	3 (1%)
1	E	278/316 (87%)	-0.07	9 (3%) 50 56	14, 33, 57, 79	3 (1%)
All	All	1395/1580 (88%)	-0.05	50 (3%) 46 52	14, 32, 62, 88	19 (1%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	-2	PHE	4.3
1	D	37	MET	4.2
1	A	-2	PHE	4.0
1	D	39	LEU	3.8
1	D	271	MET	3.3
1	D	274	GLN	3.2
1	D	273	ASP	3.1
1	A	38	ASP	3.0
1	D	-2	PHE	3.0
1	B	39	LEU	3.0
1	A	272	ALA	2.9
1	C	39	LEU	2.9
1	B	274	GLN	2.9
1	E	39	LEU	2.9
1	C	-2	PHE	2.8
1	C	38	ASP	2.8
1	D	143	VAL	2.8
1	C	143	VAL	2.8
1	A	-1	GLN	2.7
1	A	39	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	36	ASP	2.7
1	E	38	ASP	2.7
1	D	38	ASP	2.7
1	B	-4	LEU	2.7
1	E	0	SER	2.6
1	D	231	VAL	2.5
1	A	271	MET	2.5
1	D	42	VAL	2.5
1	C	-1	GLN	2.5
1	D	25	LEU	2.5
1	B	275	GLU	2.5
1	B	38	ASP	2.4
1	E	274	GLN	2.3
1	D	44	ALA	2.3
1	A	77	PHE	2.3
1	D	28	HIS	2.3
1	A	273	ASP	2.3
1	D	272	ALA	2.2
1	A	40	ALA	2.2
1	C	275	GLU	2.1
1	E	-1	GLN	2.1
1	D	40	ALA	2.1
1	A	37	MET	2.1
1	E	275	GLU	2.1
1	D	-5	ASN	2.1
1	A	36	ASP	2.0
1	B	77	PHE	2.0
1	E	77	PHE	2.0
1	E	210	LEU	2.0
1	D	77	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

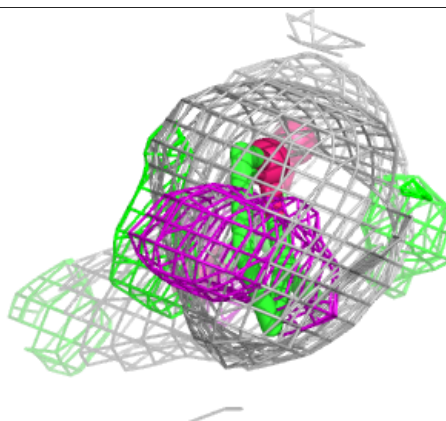
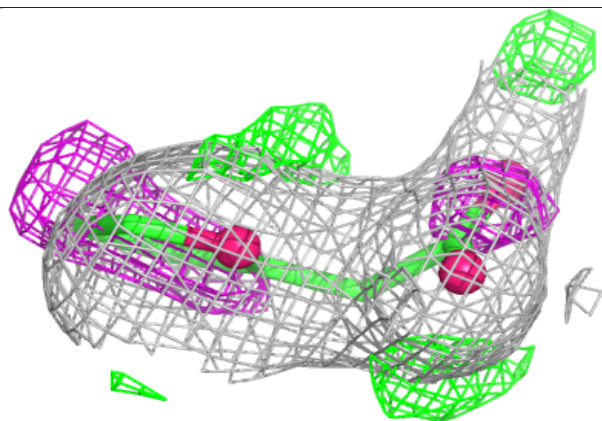
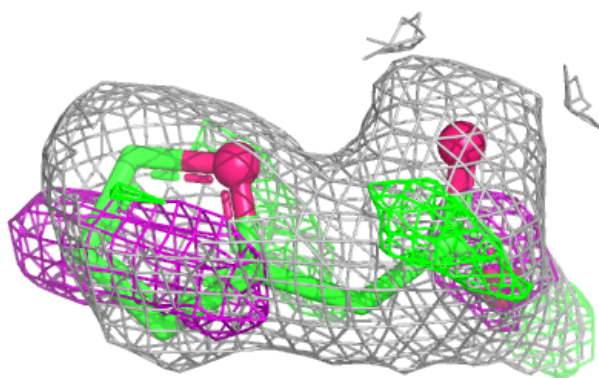
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	403	5/5	0.78	0.13	47,50,54,58	5
3	SO4	B	403	5/5	0.80	0.11	42,46,50,53	5
4	SJU	B	402[A]	9/9	0.81	0.15	30,34,37,39	9
4	SJU	B	402[B]	9/9	0.81	0.15	31,35,37,39	9
4	SJU	C	402[A]	9/9	0.81	0.15	30,36,39,39	9
4	SJU	C	402[B]	9/9	0.81	0.15	30,36,39,39	9
3	SO4	A	402	5/5	0.83	0.13	42,43,45,46	5
3	SO4	D	402	5/5	0.87	0.10	45,49,53,55	5
2	NAI	D	401	44/44	0.94	0.09	34,45,52,56	0
2	NAI	E	401	44/44	0.95	0.08	30,40,45,47	0
2	NAI	C	401	44/44	0.96	0.07	32,39,43,47	0
2	NAI	B	401	44/44	0.97	0.06	28,32,36,40	0
2	NAI	A	401	44/44	0.97	0.06	27,31,37,39	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.

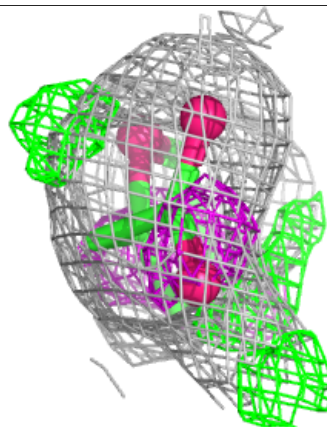
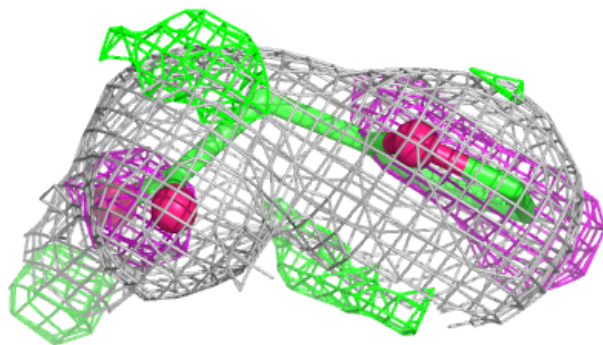
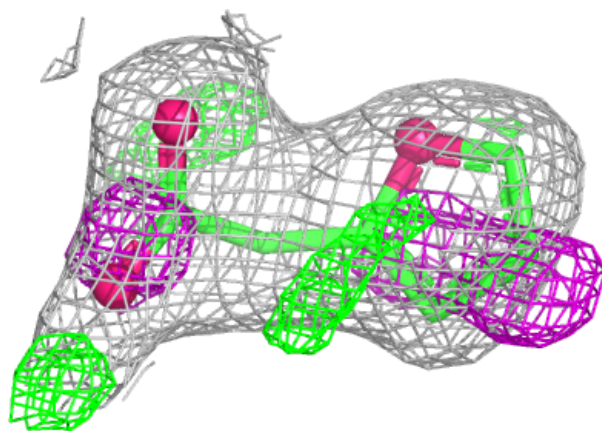
Electron density around SJU B 402 (A):

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



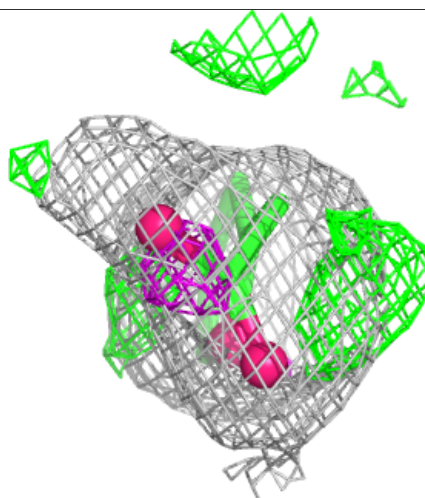
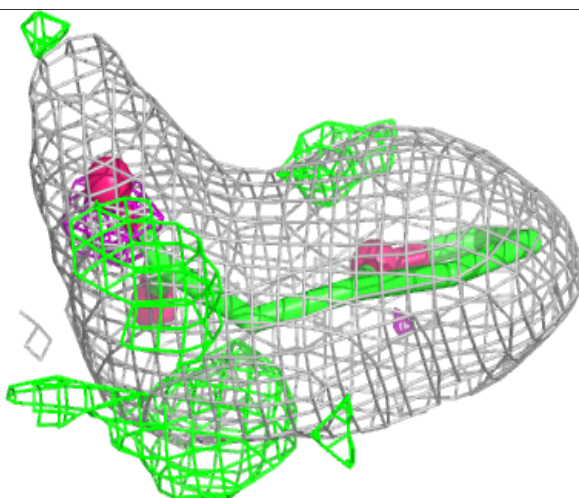
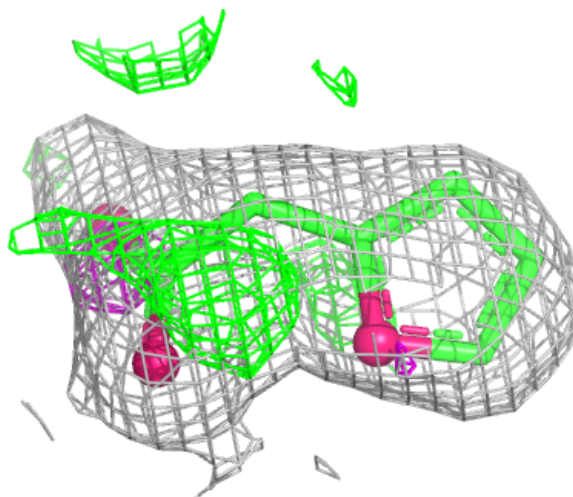
Electron density around SJU B 402 (B):

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



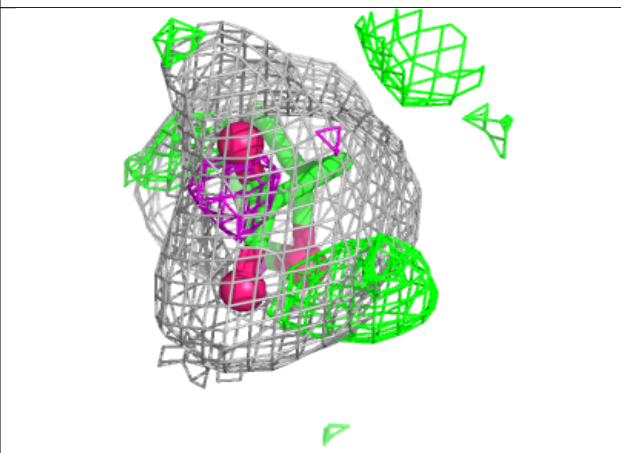
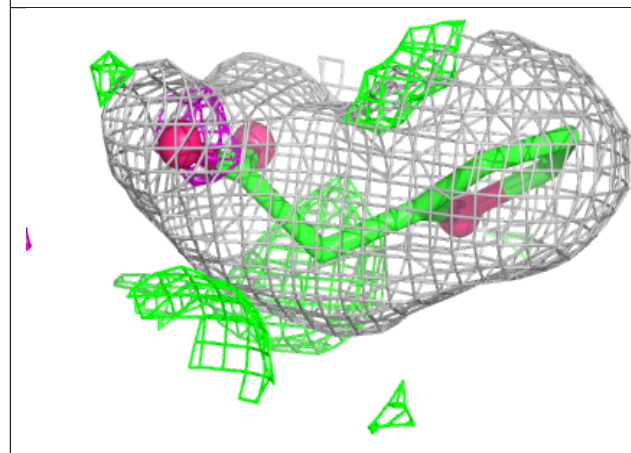
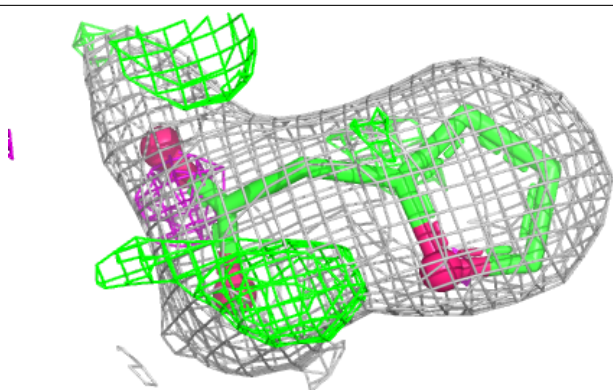
Electron density around SJU C 402 (A):

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

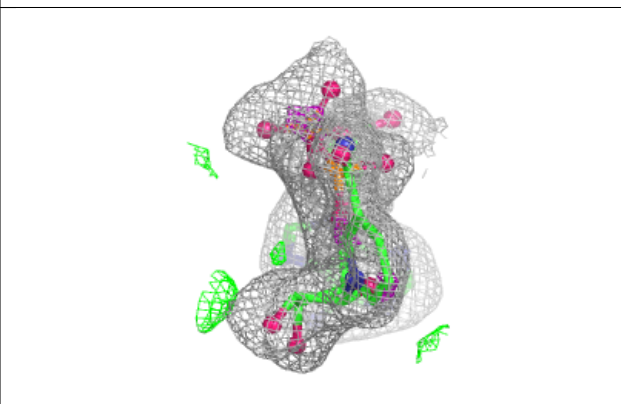
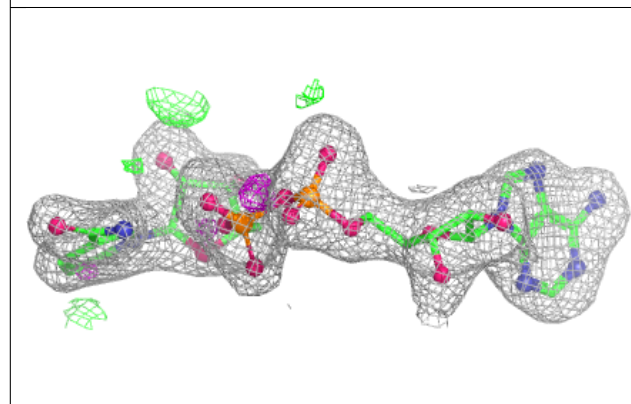
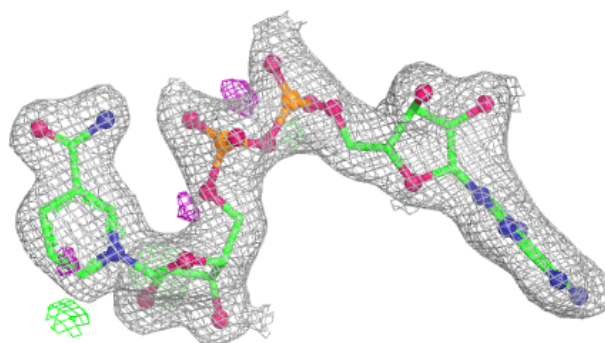


Electron density around SJU C 402 (B):

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

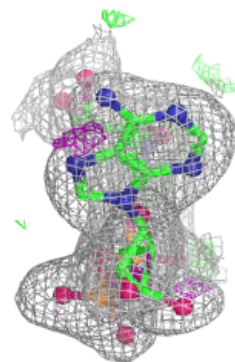
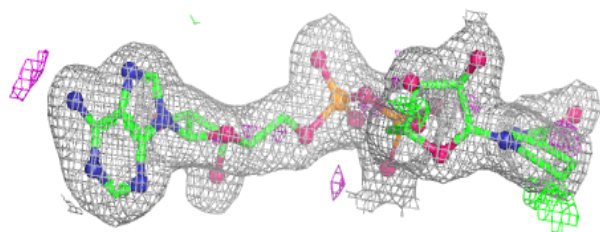
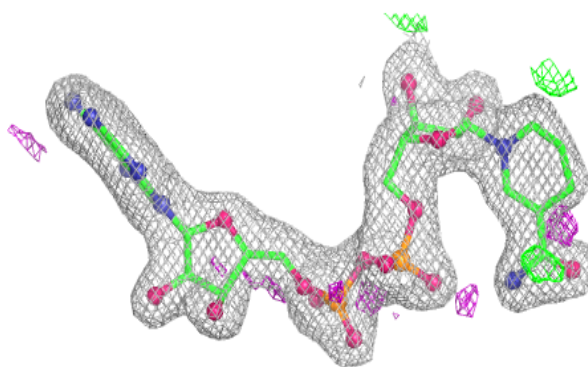
**Electron density around NAI D 401:**

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

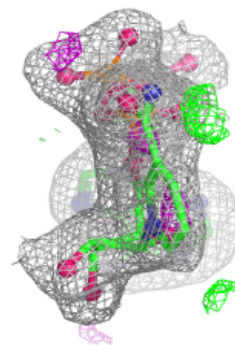
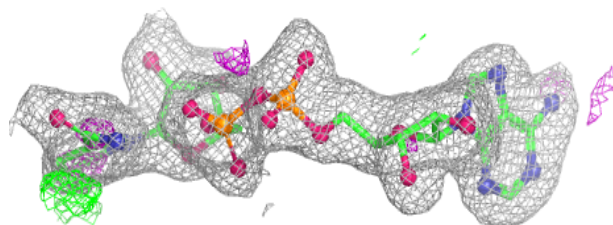
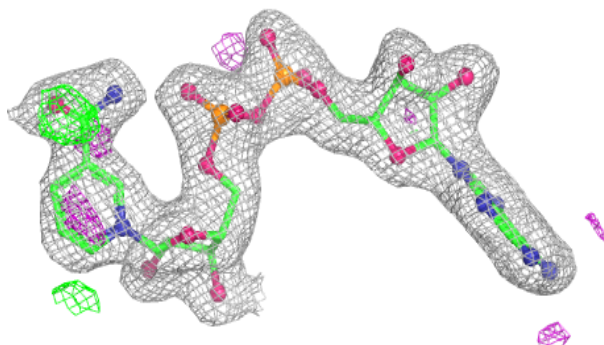


Electron density around NAI E 401:

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

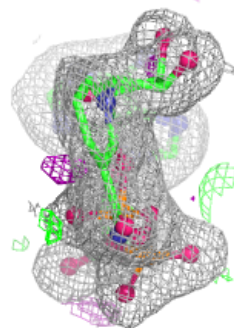
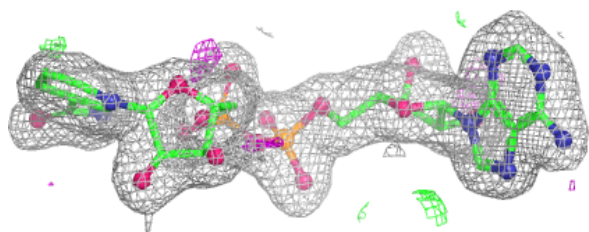
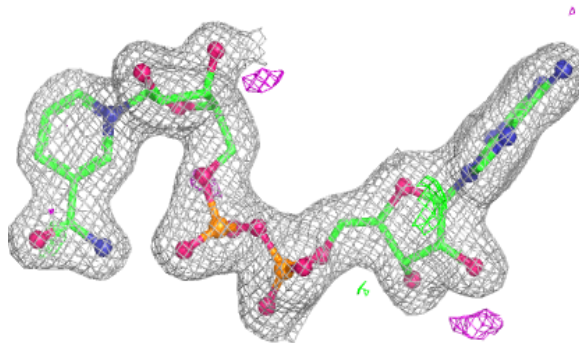
**Electron density around NAI C 401:**

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

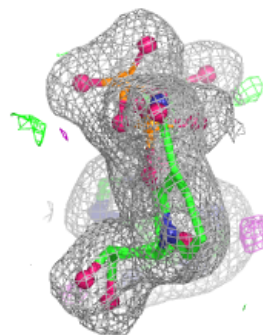
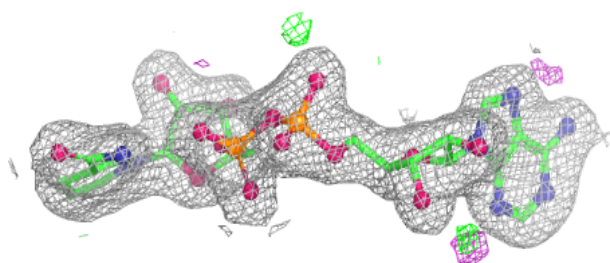
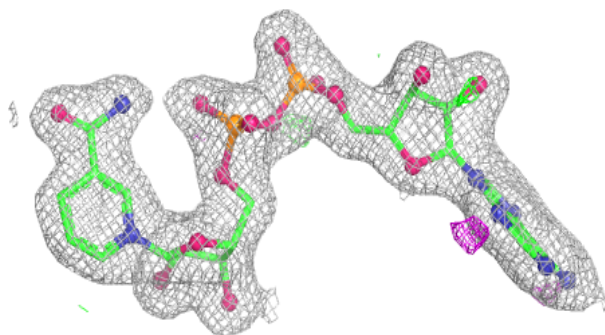


Electron density around NAI B 401:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.