



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:11 PM UTC

PDB ID : 4HCY / pdb_00004hcy
Title : Structure of a eukaryotic thiaminase-I bound to the thiamin analogue 3-deazathiamin
Authors : Kreinbring, C.A.; Hubbard, P.A.; Leeper, F.J.; Hawksley, D.; Petsko, G.A.; Ringe, D.
Deposited on : 2012-10-01
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

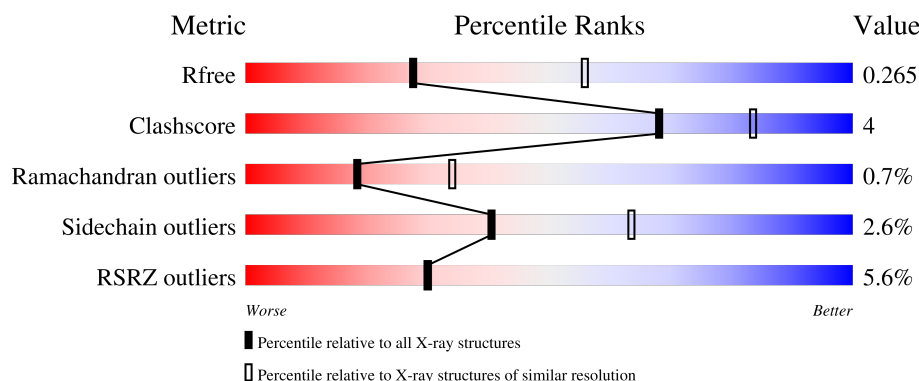
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

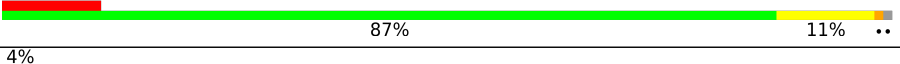
The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	357	
1	B	357	
1	C	357	
1	D	357	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	357	3% 92% 6% ..
1	F	357	4% 89% 9% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16456 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.

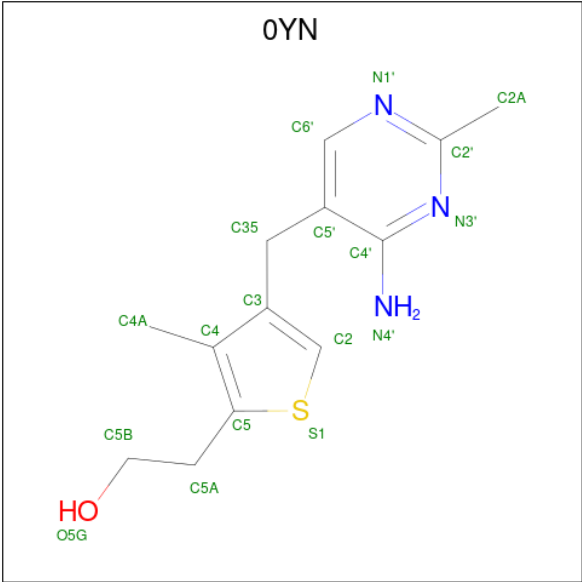
- Molecule 1 is a protein called thiaminase-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	29	0	0
			2724	1731	441	545	7			
1	B	352	Total	C	N	O	S	78	0	0
			2723	1731	441	544	7			
1	C	352	Total	C	N	O	S	31	0	0
			2723	1731	441	544	7			
1	D	352	Total	C	N	O	S	52	0	0
			2723	1731	441	544	7			
1	E	352	Total	C	N	O	S	27	1	0
			2732	1739	441	545	7			
1	F	352	Total	C	N	O	S	35	0	0
			2723	1731	441	544	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP D2V4Z5
B	0	HIS	-	expression tag	UNP D2V4Z5
C	0	HIS	-	expression tag	UNP D2V4Z5
D	0	HIS	-	expression tag	UNP D2V4Z5
E	0	HIS	-	expression tag	UNP D2V4Z5
F	0	HIS	-	expression tag	UNP D2V4Z5

- Molecule 2 is 2-{4-[(4-amino-2-methylpyrimidin-5-yl)methyl]-3-methylthiophen-2-yl}ethanol (CCD ID: 0YN) (formula: C₁₃H₁₇N₃OS).



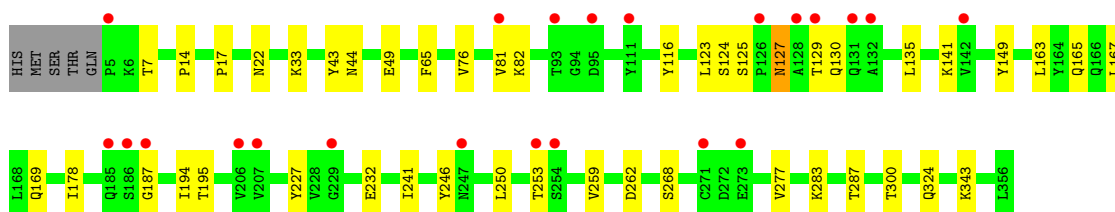
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			18	13	3	1	1		
2	B	1	Total	C	N	O	S	0	0
			18	13	3	1	1		
2	C	1	Total	C	N	O	S	0	0
			18	13	3	1	1		
2	D	1	Total	C	N	O	S	0	0
			18	13	3	1	1		
2	E	1	Total	C	N	O	S	0	0
			18	13	3	1	1		
2	F	1	Total	C	N	O	S	0	0
			18	13	3	1	1		

3 Residue-property plots [i](#)

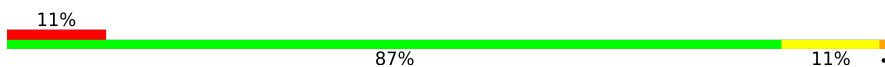
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

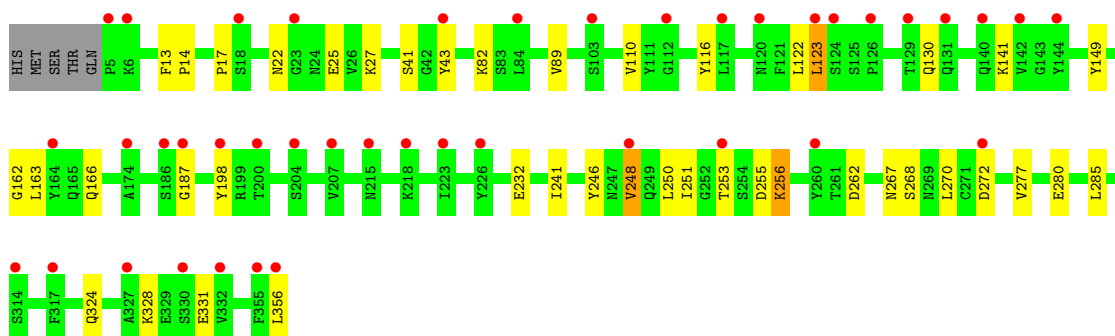
• Molecule 1: thiaminase-I

Chain A: 



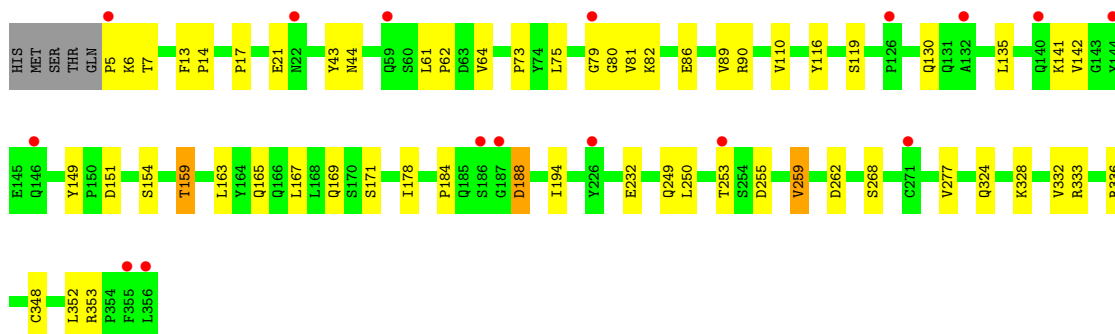
• Molecule 1: thiaminase-I

Chain B: 

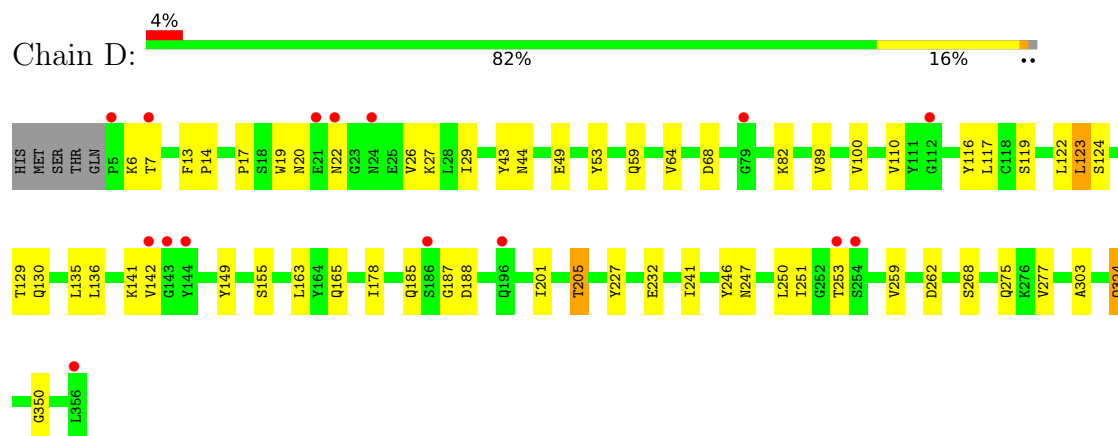


• Molecule 1: thiaminase-I

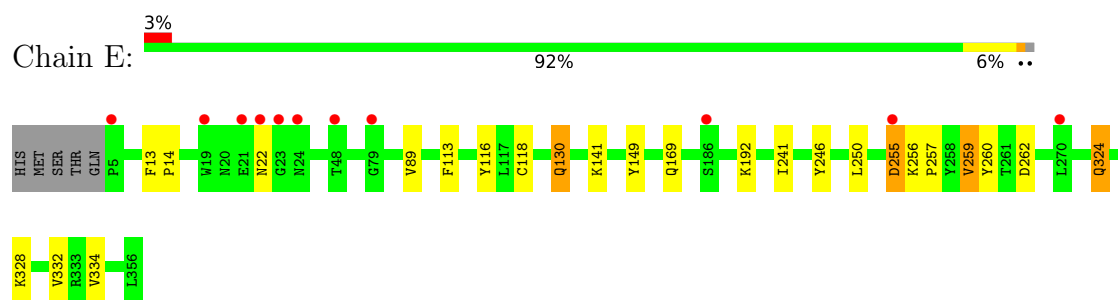
Chain C: 



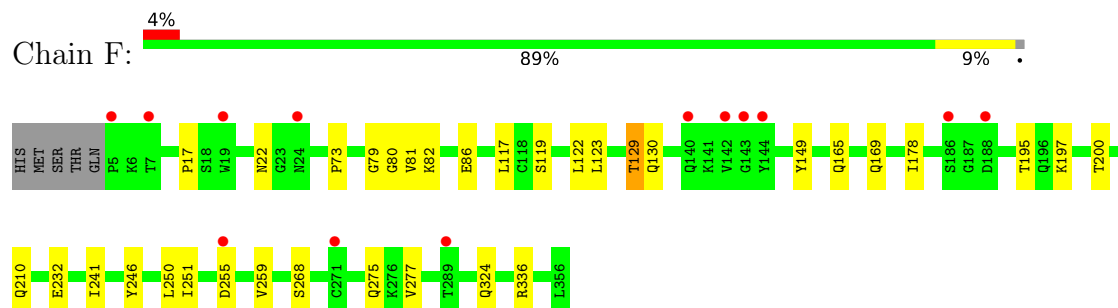
- Molecule 1: thiaminase-I



- Molecule 1: thiaminase-I



- Molecule 1: thiaminase-I



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.09Å 201.86Å 305.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.09 – 2.75 42.09 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (42.09-2.75) 98.4 (42.09-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.232 , 0.267 0.229 , 0.265	Depositor DCC
R_{free} test set	4124 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16456	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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: 0YN

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	0.26	0/2773	0.68	2/3770 (0.1%)
1	B	0.26	0/2772	0.69	2/3769 (0.1%)
1	C	0.26	0/2772	0.70	2/3769 (0.1%)
1	D	0.26	0/2772	0.70	2/3769 (0.1%)
1	E	0.26	0/2785	0.70	2/3787 (0.1%)
1	F	0.26	0/2772	0.69	2/3769 (0.1%)
All	All	0.26	0/16646	0.69	12/22633 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	TYR	CA-C-N	5.81	125.28	119.24
1	E	149	TYR	C-N-CA	5.81	125.28	119.24
1	F	149	TYR	CA-C-N	5.68	125.15	119.24
1	F	149	TYR	C-N-CA	5.68	125.15	119.24
1	C	149	TYR	CA-C-N	5.43	124.88	119.24
1	C	149	TYR	C-N-CA	5.43	124.88	119.24
1	B	149	TYR	CA-C-N	5.42	124.87	119.24
1	B	149	TYR	C-N-CA	5.42	124.87	119.24
1	A	149	TYR	CA-C-N	5.28	124.73	119.24
1	A	149	TYR	C-N-CA	5.28	124.73	119.24
1	D	149	TYR	CA-C-N	5.07	125.10	119.32
1	D	149	TYR	C-N-CA	5.07	125.10	119.32

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	2724	0	2710	19	0
1	B	2723	0	2707	19	0
1	C	2723	0	2707	28	0
1	D	2723	0	2707	28	0
1	E	2732	0	2716	12	0
1	F	2723	0	2707	11	0
2	A	18	0	17	0	0
2	B	18	0	17	0	0
2	C	18	0	17	2	0
2	D	18	0	17	1	0
2	E	18	0	17	0	0
2	F	18	0	17	0	0
All	All	16456	0	16356	117	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 4.

All (117) 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:B:17:PRO:HG3	1:B:232:GLU:HB3	1.67	0.77
1:D:250:LEU:H	1:D:324:GLN:HG2	1.49	0.76
1:A:17:PRO:HG3	1:A:232:GLU:HB3	1.69	0.74
1:C:163:LEU:HD22	1:C:253:THR:HG21	1.72	0.71
1:E:250:LEU:H	1:E:324:GLN:HG2	1.55	0.70
1:F:250:LEU:H	1:F:324:GLN:HG2	1.56	0.70
1:D:17:PRO:HG3	1:D:232:GLU:HB3	1.75	0.69
1:C:17:PRO:HG3	1:C:232:GLU:HB3	1.73	0.68
1:F:17:PRO:HG3	1:F:232:GLU:HB3	1.76	0.67
1:B:250:LEU:H	1:B:324:GLN:HG2	1.59	0.66
1:A:163:LEU:HD22	1:A:253:THR:HG21	1.79	0.65
1:C:130:GLN:HG2	1:C:141:LYS:HB3	1.79	0.65
1:D:130:GLN:HG2	1:D:141:LYS:HB3	1.77	0.64
1:C:249:GLN:HA	1:C:324:GLN:HE22	1.63	0.64
1:B:123:LEU:HD23	1:B:248:VAL:HG13	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:THR:HG22	1:D:44:ASN:HB3	1.81	0.63
1:B:256:LYS:NZ	1:B:331:GLU:OE1	2.33	0.62
1:A:250:LEU:H	1:A:324:GLN:HG2	1.66	0.60
1:C:7:THR:HG22	1:C:44:ASN:HB3	1.84	0.60
1:C:151:ASP:HB3	1:C:159:THR:HG21	1.82	0.60
1:B:82:LYS:HB2	1:B:268:SER:HA	1.83	0.60
1:F:79:GLY:O	1:F:81:VAL:N	2.36	0.59
1:C:73:PRO:HG3	1:C:336:ARG:HH11	1.69	0.58
1:B:163:LEU:HD22	1:B:253:THR:HG21	1.85	0.58
1:D:117:LEU:HG	1:D:303:ALA:HA	1.87	0.56
1:F:82:LYS:HB2	1:F:268:SER:HA	1.85	0.56
1:A:7:THR:HG22	1:A:44:ASN:HB3	1.88	0.56
1:C:353:ARG:HD2	1:D:155:SER:HB2	1.88	0.55
1:D:116:TYR:HB2	1:D:262:ASP:HB2	1.87	0.55
1:A:14:PRO:HB3	1:A:49:GLU:HB3	1.89	0.55
1:A:127:ASN:OD1	1:A:127:ASN:N	2.28	0.54
2:C:401:OYN:O5G	2:C:401:OYN:S1	2.62	0.54
1:C:82:LYS:HB2	1:C:268:SER:HA	1.89	0.54
1:B:241:ILE:HG23	1:B:246:TYR:HB2	1.91	0.53
1:C:79:GLY:O	1:C:81:VAL:N	2.39	0.53
1:A:343:LYS:NZ	1:B:25:GLU:OE2	2.41	0.53
1:C:154:SER:HB2	1:D:350:GLY:HA3	1.90	0.53
1:A:241:ILE:HG23	1:A:246:TYR:HB2	1.92	0.52
1:D:82:LYS:HB2	1:D:268:SER:HA	1.90	0.52
1:D:163:LEU:HD22	1:D:253:THR:HG21	1.90	0.52
1:D:119:SER:HB2	1:D:259:VAL:HG22	1.91	0.52
1:C:116:TYR:HB2	1:C:262:ASP:HB2	1.90	0.52
1:A:116:TYR:HB2	1:A:262:ASP:HB2	1.91	0.51
1:A:165:GLN:HG2	1:A:178:ILE:HD13	1.91	0.51
1:D:165:GLN:HG2	1:D:178:ILE:HD13	1.93	0.51
1:E:130:GLN:HG2	1:E:141:LYS:HB3	1.93	0.51
1:F:241:ILE:HG23	1:F:246:TYR:HB2	1.93	0.50
1:E:116:TYR:HB2	1:E:262:ASP:HB2	1.92	0.50
1:F:129:THR:HG22	1:F:130:GLN:HG2	1.94	0.49
1:D:135:LEU:HB2	1:D:253:THR:HA	1.93	0.49
1:C:184:PRO:HG2	1:C:352:LEU:HD21	1.95	0.49
1:D:14:PRO:HB3	1:D:49:GLU:HB3	1.94	0.49
1:D:241:ILE:HG23	1:D:246:TYR:HB2	1.95	0.49
1:A:135:LEU:HB2	1:A:253:THR:HA	1.95	0.48
1:B:130:GLN:HG2	1:B:141:LYS:HB3	1.95	0.48
1:D:122:LEU:HB2	1:D:251:ILE:HG21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:SER:OG	1:B:280:GLU:OE2	2.29	0.47
1:C:165:GLN:HG2	1:C:178:ILE:HD13	1.96	0.47
1:B:267:ASN:HB3	1:B:270:LEU:HG	1.96	0.47
1:C:249:GLN:HA	1:C:324:GLN:NE2	2.30	0.47
1:B:89:VAL:HG21	1:B:110:VAL:HG11	1.97	0.46
1:C:13:PHE:HA	1:C:14:PRO:HD3	1.77	0.46
1:D:100:VAL:HG22	1:D:117:LEU:HD21	1.97	0.46
1:F:165:GLN:HG2	1:F:178:ILE:HD13	1.96	0.46
1:A:65:PHE:HZ	1:A:81:VAL:HG12	1.80	0.46
1:D:53:TYR:OH	1:D:68:ASP:OD2	2.27	0.45
1:A:123:LEU:HB3	1:A:227:TYR:HB3	1.97	0.45
1:C:188:ASP:OD1	1:C:188:ASP:N	2.49	0.45
1:D:13:PHE:HA	1:D:14:PRO:HD3	1.77	0.45
1:C:135:LEU:HD12	1:C:253:THR:HG22	1.97	0.45
1:C:61:LEU:HA	1:C:62:PRO:HD3	1.82	0.44
1:A:130:GLN:HG2	1:A:141:LYS:HB3	1.99	0.44
1:B:43:TYR:CD1	1:B:277:VAL:HG21	2.53	0.44
1:E:13:PHE:HA	1:E:14:PRO:HD3	1.76	0.44
1:E:259:VAL:HG12	1:E:334:VAL:HG22	1.98	0.44
1:F:73:PRO:HG2	1:F:336:ARG:HB3	2.00	0.44
1:C:167:LEU:HB2	1:C:194:ILE:HG23	1.98	0.43
1:B:198:TYR:CE1	1:B:356:LEU:HD13	2.54	0.43
1:C:86:GLU:O	1:C:90:ARG:HG2	2.18	0.43
1:C:89:VAL:HG21	1:C:110:VAL:HG11	2.01	0.42
1:F:197:LYS:O	1:F:200:THR:OG1	2.34	0.42
1:B:250:LEU:O	1:B:328:LYS:NZ	2.52	0.42
1:C:119:SER:HB2	1:C:259:VAL:HG23	2.01	0.42
1:E:241:ILE:HG23	1:E:246:TYR:HB2	2.01	0.42
1:C:328:LYS:O	1:C:332:VAL:HG23	2.19	0.42
1:D:123:LEU:HB3	1:D:227:TYR:HB3	2.00	0.42
1:C:171:SER:O	1:C:333:ARG:NH2	2.52	0.42
1:D:124:SER:HB2	1:D:247:ASN:HB2	2.00	0.42
1:A:167:LEU:HB2	1:A:194:ILE:HG23	2.01	0.42
1:B:13:PHE:HA	1:B:14:PRO:HD3	1.86	0.42
1:D:43:TYR:CD1	1:D:277:VAL:HG21	2.55	0.42
1:C:43:TYR:CD1	1:C:277:VAL:HG21	2.55	0.41
1:D:89:VAL:HG21	1:D:110:VAL:HG11	2.01	0.41
1:A:43:TYR:CD1	1:A:277:VAL:HG21	2.55	0.41
1:A:82:LYS:HB2	1:A:268:SER:HA	2.03	0.41
1:D:19:TRP:HB2	1:D:26:VAL:HB	2.03	0.41
1:C:184:PRO:HD2	1:C:348:CYS:SG	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:ASP:OD2	1:E:256:LYS:NZ	2.49	0.41
1:E:328:LYS:O	1:E:332:VAL:HG23	2.21	0.41
1:D:201:ILE:O	1:D:205:THR:HG22	2.20	0.41
1:E:89:VAL:HA	1:E:113:PHE:CE2	2.56	0.41
1:A:283:LYS:O	1:A:287:THR:OG1	2.33	0.41
1:B:116:TYR:HB2	1:B:262:ASP:HB2	2.02	0.41
1:B:162:GLY:O	1:B:166:GLN:HG3	2.21	0.41
1:E:256:LYS:HA	1:E:257:PRO:HD3	1.93	0.41
1:D:27:LYS:HB3	1:D:29:ILE:HG22	2.02	0.41
1:F:122:LEU:HB2	1:F:251:ILE:HG21	2.03	0.41
2:C:401:OYN:H16	2:C:401:OYN:H5	1.76	0.40
1:D:6:LYS:HB3	1:D:43:TYR:CE2	2.56	0.40
1:D:136:LEU:HD23	1:D:136:LEU:HA	1.95	0.40
1:F:119:SER:HB2	1:F:259:VAL:HG12	2.02	0.40
1:B:122:LEU:HB2	1:B:251:ILE:HG21	2.03	0.40
1:A:76:VAL:HG22	1:A:81:VAL:HG21	2.03	0.40
2:D:401:OYN:H16	2:D:401:OYN:H5	1.78	0.40
1:E:130:GLN:CG	1:E:141:LYS:HB3	2.52	0.40
1:C:5:PRO:HB2	1:C:6:LYS:H	1.63	0.40
1:E:118:CYS:HB3	1:E:260:TYR:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	350/357 (98%)	331 (95%)	17 (5%)	2 (1%)	21	38
1	B	350/357 (98%)	329 (94%)	18 (5%)	3 (1%)	14	28
1	C	350/357 (98%)	336 (96%)	12 (3%)	2 (1%)	21	38
1	D	350/357 (98%)	336 (96%)	12 (3%)	2 (1%)	21	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	351/357 (98%)	337 (96%)	12 (3%)	2 (1%)	21	38
1	F	350/357 (98%)	336 (96%)	11 (3%)	3 (1%)	14	28
All	All	2101/2142 (98%)	2005 (95%)	82 (4%)	14 (1%)	18	34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	80	GLY
1	C	80	GLY
1	C	255	ASP
1	E	22	ASN
1	F	255	ASP
1	A	22	ASN
1	B	22	ASN
1	B	255	ASP
1	D	22	ASN
1	E	255	ASP
1	F	22	ASN
1	B	187	GLY
1	D	187	GLY
1	A	187	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	314/319 (98%)	305 (97%)	9 (3%)	37	61
1	B	313/319 (98%)	307 (98%)	6 (2%)	50	70
1	C	313/319 (98%)	304 (97%)	9 (3%)	37	61
1	D	313/319 (98%)	302 (96%)	11 (4%)	32	56
1	E	314/319 (98%)	309 (98%)	5 (2%)	55	73
1	F	313/319 (98%)	304 (97%)	9 (3%)	37	61
All	All	1880/1914 (98%)	1831 (97%)	49 (3%)	40	63

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	124	SER
1	A	125	SER
1	A	127	ASN
1	A	129	THR
1	A	169	GLN
1	A	195	THR
1	A	259	VAL
1	A	300	THR
1	B	27	LYS
1	B	123	LEU
1	B	248	VAL
1	B	256	LYS
1	B	272	ASP
1	B	285	LEU
1	C	21	GLU
1	C	64	VAL
1	C	75	LEU
1	C	142	VAL
1	C	159	THR
1	C	169	GLN
1	C	188	ASP
1	C	250	LEU
1	C	259	VAL
1	D	20	ASN
1	D	59	GLN
1	D	64	VAL
1	D	123	LEU
1	D	129	THR
1	D	142	VAL
1	D	185	GLN
1	D	188	ASP
1	D	205	THR
1	D	275	GLN
1	D	324	GLN
1	E	130	GLN
1	E	169	GLN
1	E	192	LYS
1	E	259	VAL
1	E	324	GLN
1	F	86	GLU
1	F	117	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	123	LEU
1	F	129	THR
1	F	169	GLN
1	F	195	THR
1	F	210	GLN
1	F	275	GLN
1	F	277	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	247	ASN
1	A	320	GLN
1	B	24	ASN
1	B	166	GLN
1	B	247	ASN
1	B	320	GLN
1	C	39	GLN
1	C	44	ASN
1	C	120	ASN
1	C	166	GLN
1	C	210	GLN
1	C	249	GLN
1	D	59	GLN
1	D	97	HIS
1	D	120	ASN
1	D	247	ASN
1	D	249	GLN
1	D	320	GLN
1	E	24	ASN
1	E	120	ASN
1	F	59	GLN
1	F	97	HIS
1	F	120	ASN
1	F	189	GLN
1	F	245	GLN
1	F	247	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	0YN	E	401	-	18,19,19	1.43	2 (11%)	25,26,26	2.11	11 (44%)
2	0YN	F	401	-	18,19,19	1.40	2 (11%)	25,26,26	2.14	11 (44%)
2	0YN	B	401	-	18,19,19	1.43	2 (11%)	25,26,26	2.13	11 (44%)
2	0YN	A	401	-	18,19,19	1.38	2 (11%)	25,26,26	2.22	12 (48%)
2	0YN	D	401	-	18,19,19	1.42	2 (11%)	25,26,26	2.11	11 (44%)
2	0YN	C	401	-	18,19,19	1.45	2 (11%)	25,26,26	2.12	11 (44%)

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	0YN	E	401	-	-	0/7/7/7	0/2/2/2
2	0YN	F	401	-	-	0/7/7/7	0/2/2/2
2	0YN	B	401	-	-	0/7/7/7	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0YN	A	401	-	-	2/7/7/7	0/2/2/2
2	0YN	D	401	-	-	0/7/7/7	0/2/2/2
2	0YN	C	401	-	-	0/7/7/7	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	0YN	C2-C3	5.01	1.41	1.36
2	E	401	0YN	C2-C3	4.96	1.41	1.36
2	D	401	0YN	C2-C3	4.92	1.41	1.36
2	B	401	0YN	C2-C3	4.88	1.41	1.36
2	F	401	0YN	C2-C3	4.83	1.41	1.36
2	A	401	0YN	C2-C3	4.71	1.40	1.36
2	B	401	0YN	C5'-C4'	-2.64	1.38	1.42
2	E	401	0YN	C5'-C4'	-2.64	1.38	1.42
2	F	401	0YN	C5'-C4'	-2.64	1.38	1.42
2	C	401	0YN	C5'-C4'	-2.64	1.38	1.42
2	A	401	0YN	C5'-C4'	-2.62	1.38	1.42
2	D	401	0YN	C5'-C4'	-2.60	1.38	1.42

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	0YN	C2-C3-C4	4.22	114.90	111.92
2	F	401	0YN	C2-C3-C4	4.04	114.77	111.92
2	B	401	0YN	C2-C3-C4	4.00	114.74	111.92
2	E	401	0YN	C2-C3-C4	3.80	114.60	111.92
2	D	401	0YN	C2-C3-C4	3.80	114.60	111.92
2	C	401	0YN	C2-C3-C4	3.79	114.60	111.92
2	A	401	0YN	C5A-C5-C4	3.73	135.74	130.78
2	B	401	0YN	C3-C2-S1	-3.46	109.56	113.46
2	A	401	0YN	C3-C2-S1	-3.43	109.60	113.46
2	C	401	0YN	C2-S1-C5	3.42	95.64	92.41
2	C	401	0YN	C3-C2-S1	-3.42	109.61	113.46
2	D	401	0YN	C2-S1-C5	3.41	95.63	92.41
2	F	401	0YN	C3-C2-S1	-3.39	109.64	113.46
2	D	401	0YN	C3-C2-S1	-3.38	109.65	113.46
2	E	401	0YN	C3-C2-S1	-3.36	109.67	113.46
2	A	401	0YN	C2-S1-C5	3.35	95.58	92.41
2	B	401	0YN	C2-S1-C5	3.33	95.55	92.41
2	F	401	0YN	C2-S1-C5	3.32	95.54	92.41
2	E	401	0YN	C2-S1-C5	3.29	95.52	92.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	0YN	N1'-C2'-N3'	-3.01	120.52	125.53
2	A	401	0YN	N1'-C2'-N3'	-3.00	120.53	125.53
2	E	401	0YN	N1'-C2'-N3'	-3.00	120.53	125.53
2	D	401	0YN	N1'-C2'-N3'	-3.00	120.53	125.53
2	B	401	0YN	N1'-C2'-N3'	-2.97	120.60	125.53
2	F	401	0YN	C5A-C5-C4	2.96	134.71	130.78
2	F	401	0YN	N1'-C2'-N3'	-2.95	120.62	125.53
2	E	401	0YN	C35-C3-C4	-2.91	121.08	126.31
2	C	401	0YN	C35-C3-C4	-2.90	121.10	126.31
2	B	401	0YN	C35-C3-C4	-2.90	121.11	126.31
2	C	401	0YN	C6'-N1'-C2'	2.85	120.75	116.07
2	D	401	0YN	C5A-C5-C4	2.84	134.56	130.78
2	E	401	0YN	C6'-N1'-C2'	2.84	120.73	116.07
2	F	401	0YN	C6'-C5'-C4'	2.84	119.03	115.55
2	A	401	0YN	C6'-N1'-C2'	2.83	120.72	116.07
2	F	401	0YN	C6'-N1'-C2'	2.83	120.72	116.07
2	D	401	0YN	C6'-N1'-C2'	2.83	120.72	116.07
2	B	401	0YN	C6'-N1'-C2'	2.82	120.70	116.07
2	B	401	0YN	C6'-C5'-C4'	2.81	119.00	115.55
2	A	401	0YN	C6'-C5'-C4'	2.81	119.00	115.55
2	D	401	0YN	C35-C3-C4	-2.75	121.38	126.31
2	C	401	0YN	C5A-C5-C4	2.75	134.43	130.78
2	E	401	0YN	C6'-C5'-C4'	2.73	118.90	115.55
2	F	401	0YN	C35-C3-C4	-2.69	121.49	126.31
2	D	401	0YN	C6'-C5'-C4'	2.69	118.85	115.55
2	E	401	0YN	C5A-C5-C4	2.67	134.33	130.78
2	C	401	0YN	C6'-C5'-C4'	2.65	118.81	115.55
2	B	401	0YN	C5A-C5-C4	2.62	134.25	130.78
2	B	401	0YN	C5'-C6'-N1'	-2.57	119.66	123.83
2	F	401	0YN	C5'-C6'-N1'	-2.57	119.66	123.83
2	A	401	0YN	C5'-C6'-N1'	-2.54	119.69	123.83
2	E	401	0YN	C5'-C6'-N1'	-2.54	119.71	123.83
2	C	401	0YN	C5'-C6'-N1'	-2.51	119.75	123.83
2	D	401	0YN	C5'-C6'-N1'	-2.48	119.80	123.83
2	C	401	0YN	C2A-C2'-N1'	2.43	119.79	117.20
2	F	401	0YN	C2A-C2'-N1'	2.42	119.78	117.20
2	D	401	0YN	C2A-C2'-N1'	2.41	119.77	117.20
2	E	401	0YN	C2A-C2'-N1'	2.41	119.76	117.20
2	A	401	0YN	N4'-C4'-N3'	2.37	120.22	117.03
2	B	401	0YN	C2A-C2'-N1'	2.36	119.71	117.20
2	B	401	0YN	N4'-C4'-N3'	2.35	120.19	117.03
2	A	401	0YN	C2A-C2'-N1'	2.34	119.70	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	0YN	N4'-C4'-N3'	2.34	120.18	117.03
2	D	401	0YN	N4'-C4'-N3'	2.32	120.16	117.03
2	E	401	0YN	N4'-C4'-N3'	2.32	120.16	117.03
2	A	401	0YN	C35-C3-C4	-2.30	122.18	126.31
2	C	401	0YN	N4'-C4'-N3'	2.27	120.09	117.03
2	A	401	0YN	C5A-C5-S1	-2.04	116.13	120.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	0YN	C4-C5-C5A-C5B
2	A	401	0YN	S1-C5-C5A-C5B

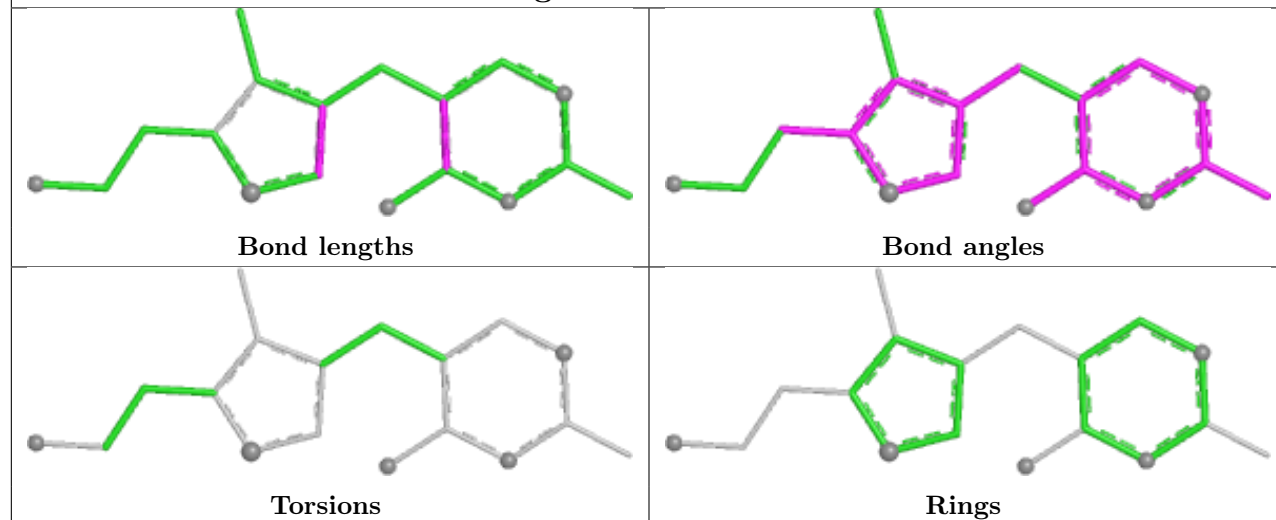
There are no ring outliers.

2 monomers are involved in 3 short contacts:

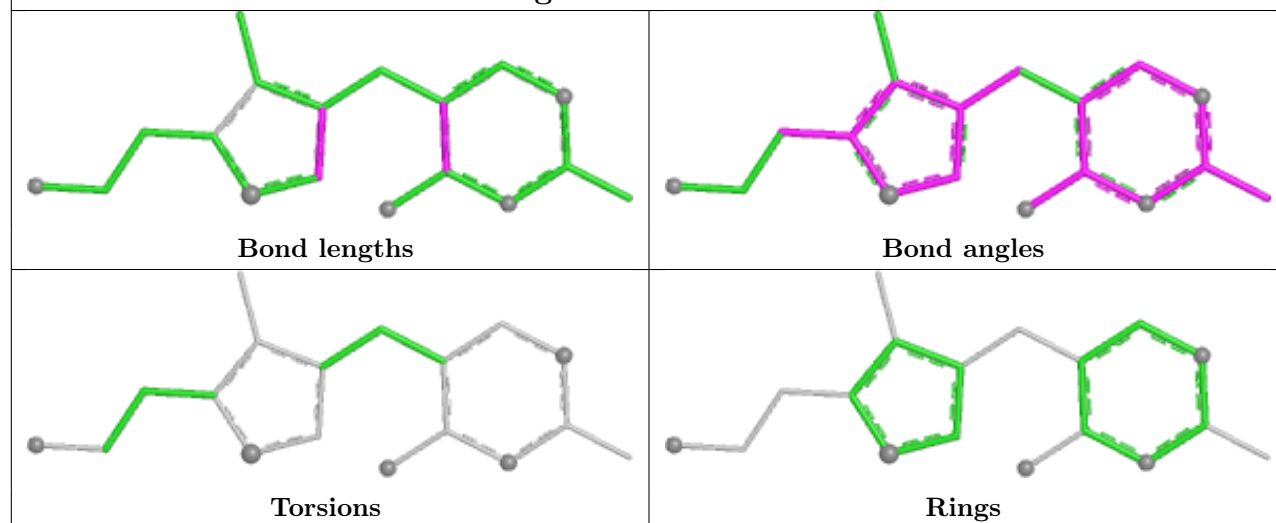
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	0YN	1	0
2	C	401	0YN	2	0

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

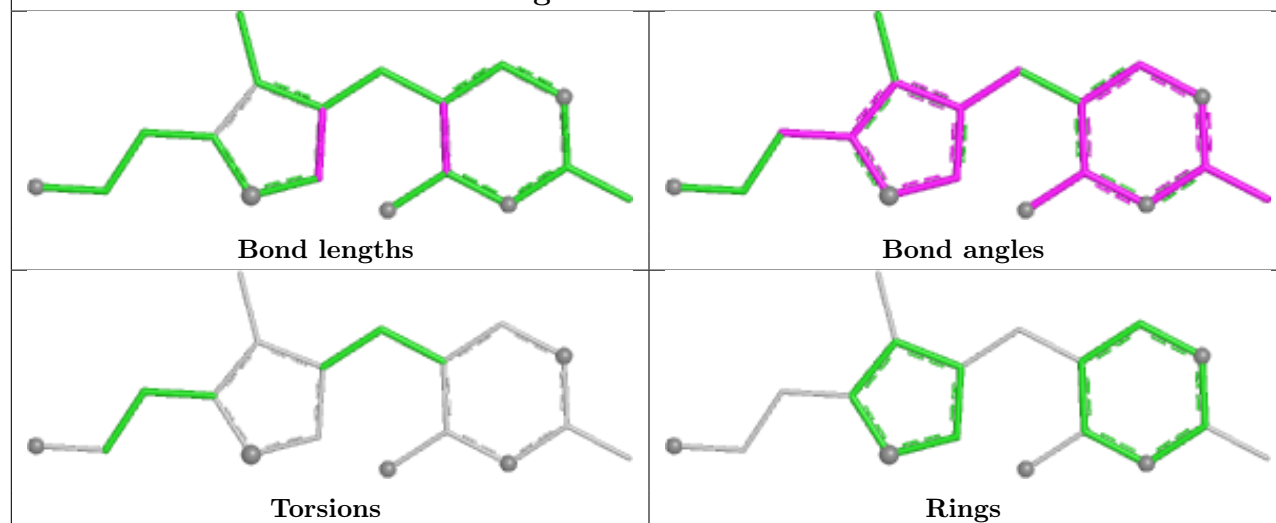
Ligand 0YN E 401



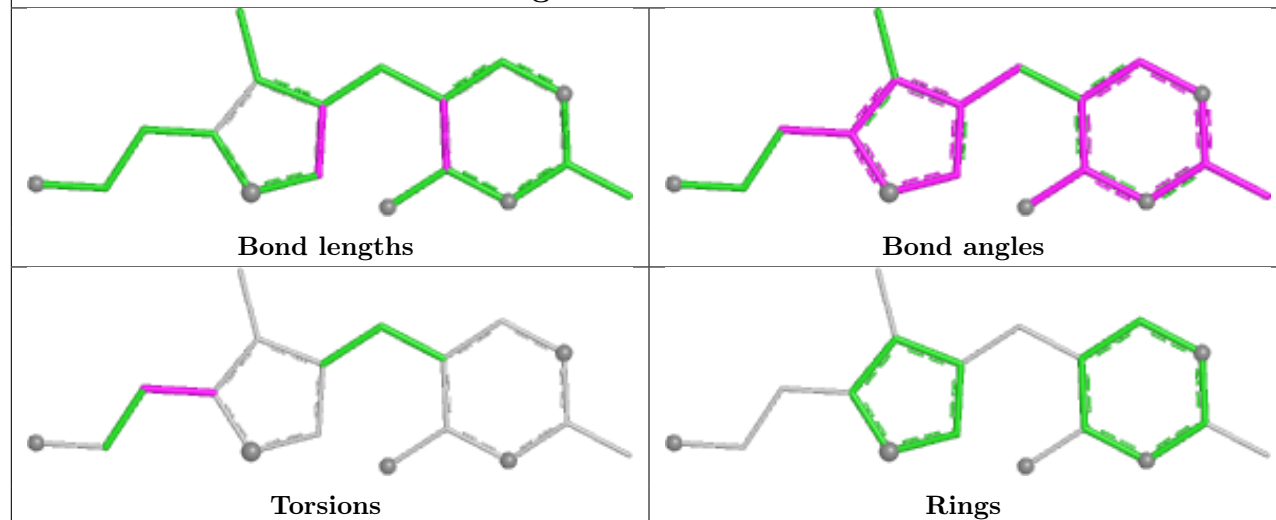
Ligand 0YN F 401



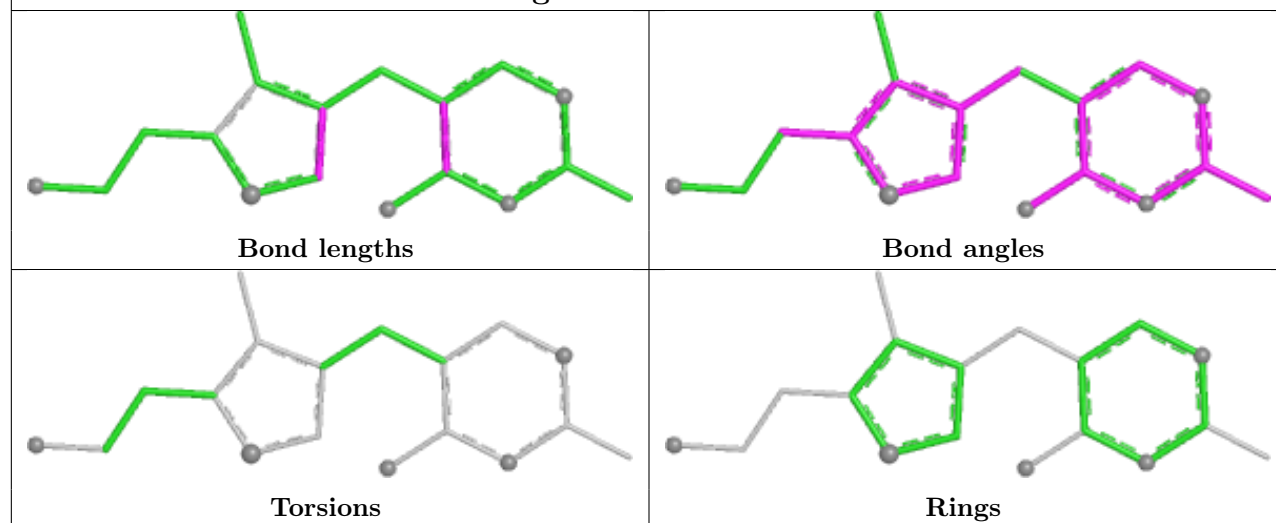
Ligand 0YN B 401



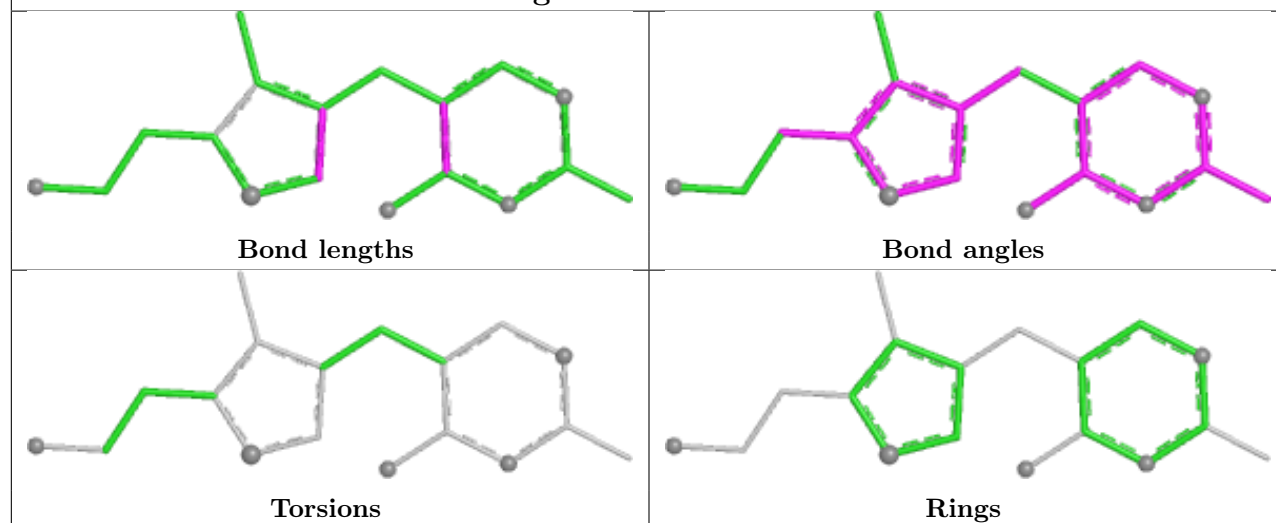
Ligand 0YN A 401



Ligand 0YN D 401



Ligand 0YN C 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	352/357 (98%)	0.67	22 (6%) 26 26	36, 69, 109, 182	9 (2%)
1	B	352/357 (98%)	0.94	41 (11%) 9 8	34, 82, 120, 158	21 (5%)
1	C	352/357 (98%)	0.46	16 (4%) 38 37	21, 62, 104, 162	11 (3%)
1	D	352/357 (98%)	0.39	15 (4%) 40 38	26, 63, 103, 144	15 (4%)
1	E	352/357 (98%)	0.25	11 (3%) 51 49	25, 57, 102, 171	10 (2%)
1	F	352/357 (98%)	0.50	13 (3%) 45 42	14, 66, 100, 182	8 (2%)
All	All	2112/2142 (98%)	0.54	118 (5%) 30 30	14, 65, 109, 182	74 (3%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	144	TYR	5.6
1	A	5	PRO	4.8
1	C	5	PRO	4.3
1	E	5	PRO	4.2
1	D	143	GLY	4.2
1	B	186	SER	4.1
1	B	253	THR	4.1
1	D	186	SER	3.9
1	D	5	PRO	3.9
1	B	5	PRO	3.8
1	B	272	ASP	3.7
1	A	129	THR	3.7
1	E	48	THR	3.7
1	A	271	CYS	3.7
1	E	79	GLY	3.7
1	A	142	VAL	3.6
1	B	174	ALA	3.5
1	F	142	VAL	3.4
1	C	22	ASN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	253	THR	3.3
1	B	103	SER	3.3
1	C	79	GLY	3.2
1	C	126	PRO	3.2
1	B	142	VAL	3.2
1	E	24	ASN	3.2
1	A	187	GLY	3.2
1	A	207	VAL	3.2
1	C	253	THR	3.1
1	E	23	GLY	3.1
1	B	140	GLN	3.1
1	E	186	SER	3.1
1	F	24	ASN	3.0
1	E	22	ASN	3.0
1	F	144	TYR	3.0
1	A	128	ALA	3.0
1	B	6	LYS	2.9
1	B	18	SER	2.9
1	C	186	SER	2.9
1	B	23	GLY	2.8
1	D	144	TYR	2.8
1	B	327	ALA	2.8
1	B	207	VAL	2.8
1	A	126	PRO	2.7
1	F	5	PRO	2.7
1	A	81	VAL	2.7
1	A	131	GLN	2.7
1	F	186	SER	2.7
1	A	206	VAL	2.7
1	B	355	PHE	2.7
1	B	144	TYR	2.6
1	E	270	LEU	2.6
1	B	215	ASN	2.6
1	A	95	ASP	2.6
1	B	43	TYR	2.6
1	D	254	SER	2.6
1	D	21	GLU	2.6
1	E	255	ASP	2.5
1	F	143	GLY	2.5
1	D	196	GLN	2.5
1	B	124	SER	2.5
1	F	271	CYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	187	GLY	2.5
1	A	273	GLU	2.5
1	A	111	TYR	2.5
1	D	79	GLY	2.4
1	F	255	ASP	2.4
1	A	254	SER	2.4
1	C	132	ALA	2.4
1	B	84	LEU	2.4
1	E	19	TRP	2.4
1	C	187	GLY	2.4
1	C	226	TYR	2.3
1	B	204	SER	2.3
1	B	226	TYR	2.3
1	A	185	GLN	2.3
1	D	356	LEU	2.3
1	D	7	THR	2.3
1	F	19	TRP	2.3
1	D	112	GLY	2.3
1	D	22	ASN	2.3
1	C	59	GLN	2.3
1	C	146	GLN	2.3
1	D	142	VAL	2.3
1	C	355	PHE	2.3
1	B	200	THR	2.2
1	F	289	THR	2.2
1	A	186	SER	2.2
1	B	120	ASN	2.2
1	C	140	GLN	2.2
1	B	117	LEU	2.2
1	A	93	THR	2.2
1	D	253	THR	2.2
1	B	112	GLY	2.2
1	B	248	VAL	2.2
1	F	7	THR	2.2
1	A	247	ASN	2.2
1	B	198	TYR	2.2
1	B	332	VAL	2.2
1	C	271	CYS	2.1
1	B	126	PRO	2.1
1	B	131	GLN	2.1
1	B	164	TYR	2.1
1	B	123	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	188	ASP	2.1
1	B	218	LYS	2.1
1	B	330	SER	2.1
1	E	21	GLU	2.1
1	B	129	THR	2.1
1	B	356	LEU	2.1
1	A	229	GLY	2.1
1	B	223	ILE	2.1
1	A	132	ALA	2.1
1	D	24	ASN	2.1
1	B	317	PHE	2.1
1	B	314	SER	2.0
1	C	356	LEU	2.0
1	F	140	GLN	2.0
1	B	260	TYR	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 oligosaccharides in this entry.

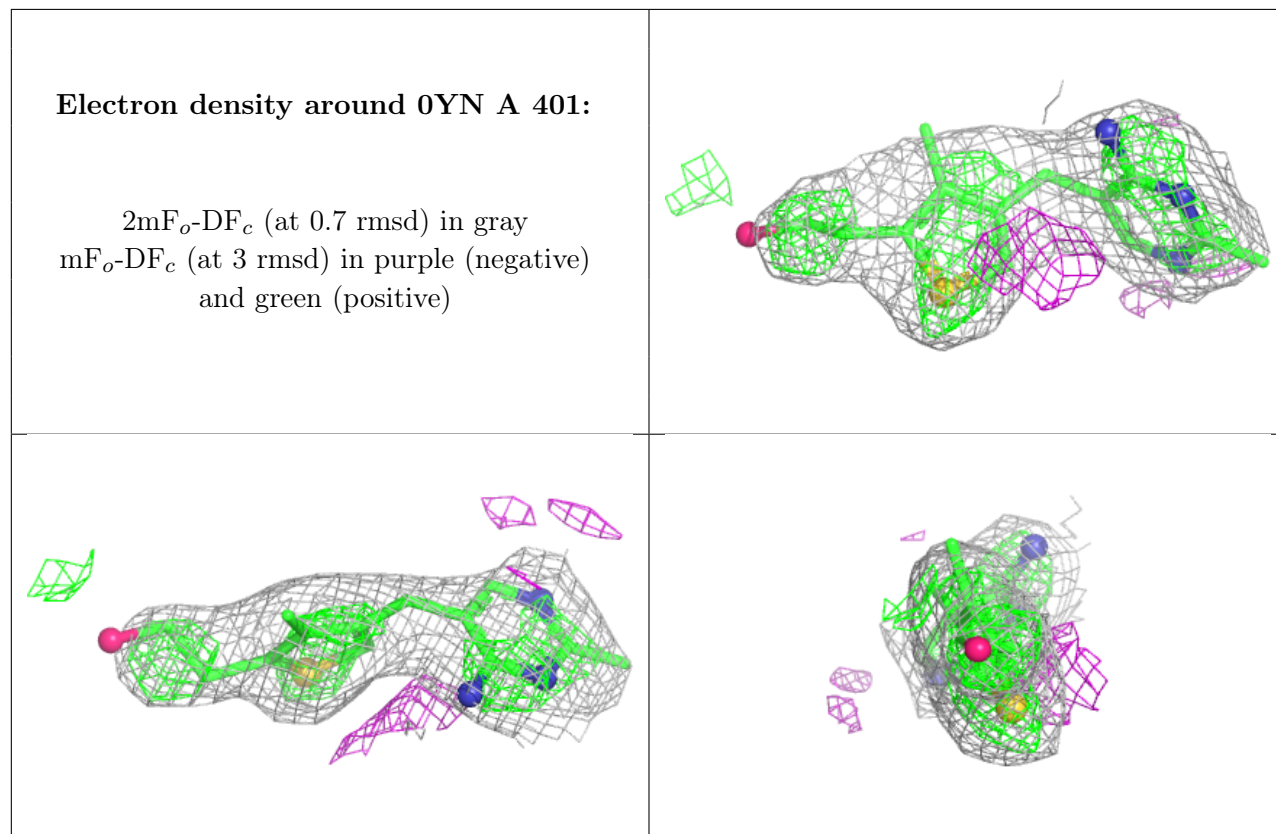
6.4 Ligands [i](#)

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
2	0YN	A	401	18/18	0.91	0.32	128,128,128,128	0
2	0YN	C	401	18/18	0.92	0.29	128,128,128,128	0
2	0YN	B	401	18/18	0.93	0.26	128,128,128,128	0
2	0YN	D	401	18/18	0.93	0.31	128,128,128,128	0
2	0YN	E	401	18/18	0.93	0.34	128,128,128,128	0
2	0YN	F	401	18/18	0.93	0.30	128,128,128,128	0

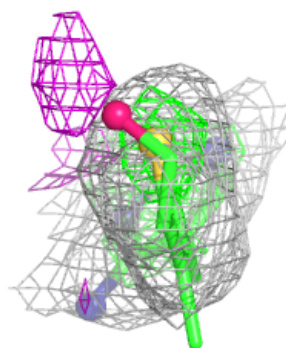
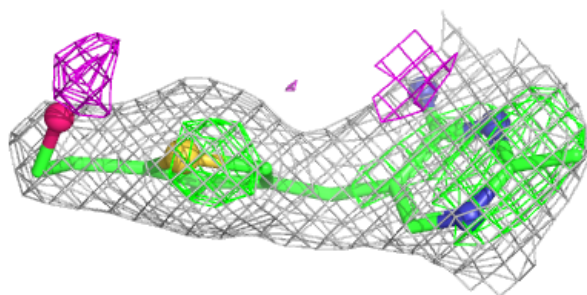
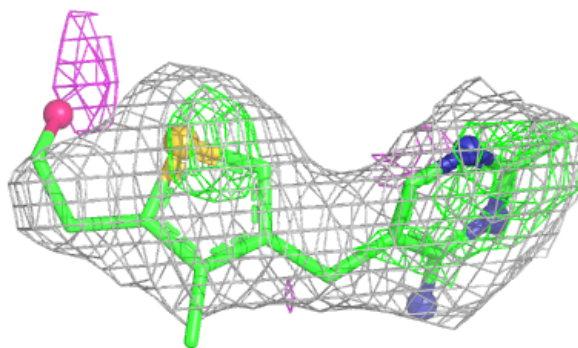
The following is a graphical depiction of the model fit to experimental electron density of all

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.

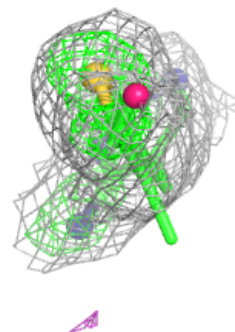
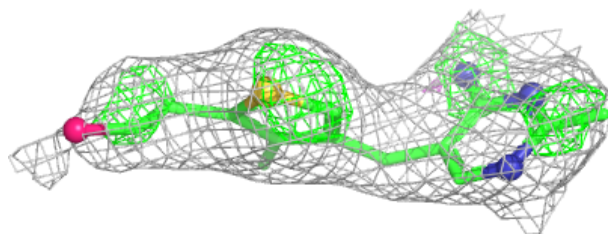
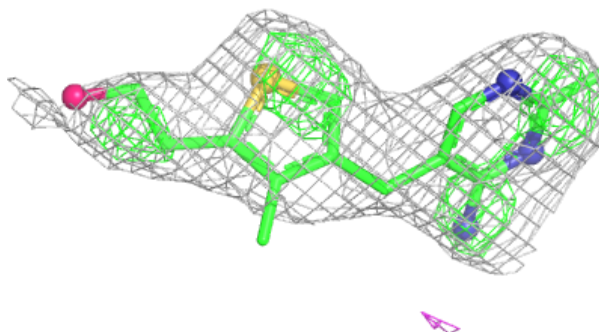


Electron density around 0YN C 401:

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

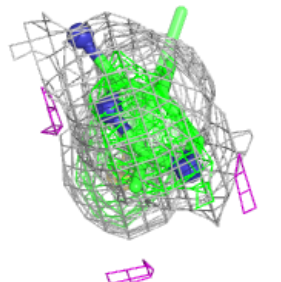
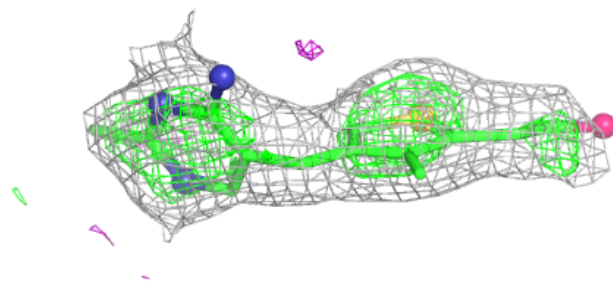
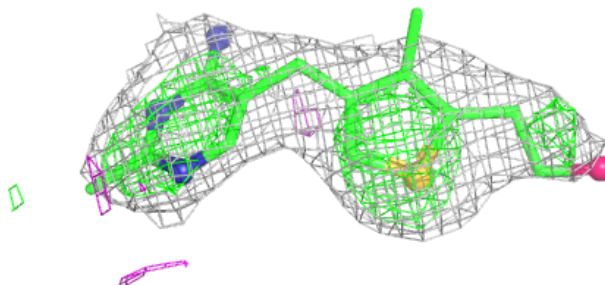
**Electron density around 0YN B 401:**

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

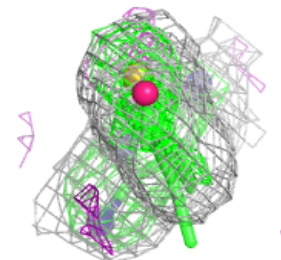
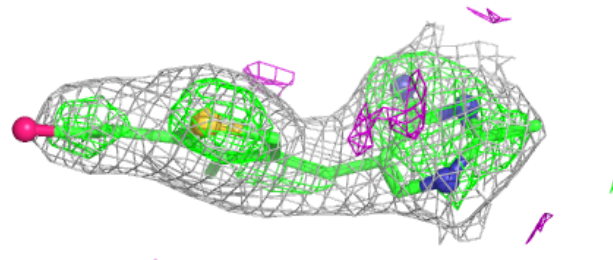
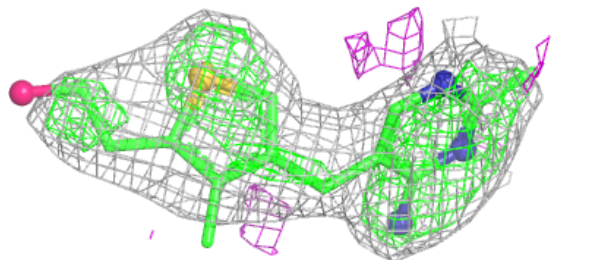


Electron density around 0YN D 401:

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

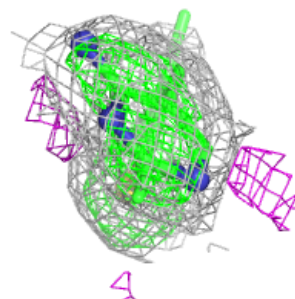
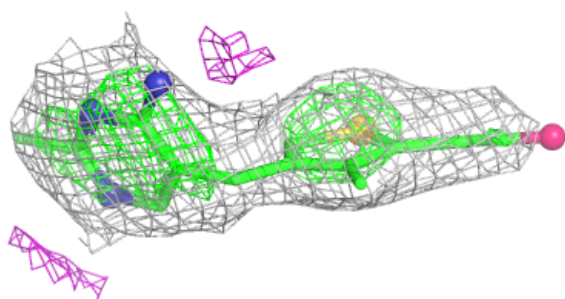
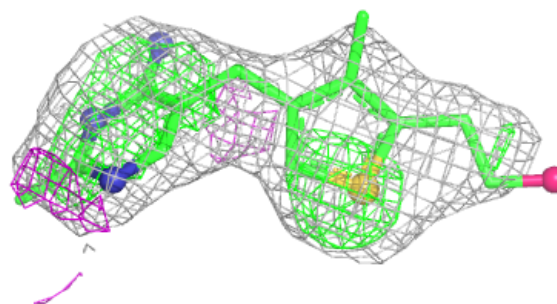
**Electron density around 0YN E 401:**

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



Electron density around 0YN F 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 ⓘ

There are no such residues in this entry.