



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:06 PM UTC

PDB ID : 9ISR / pdb_00009isr
Title : Human MTHFD1 in complex with compound 16g
Authors : Lee, L.C.; Wu, S.Y.
Deposited on : 2024-07-18
Resolution : 2.50 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

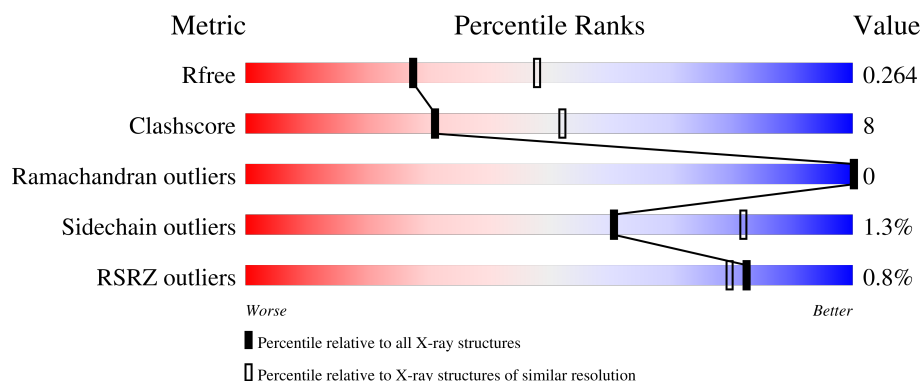
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

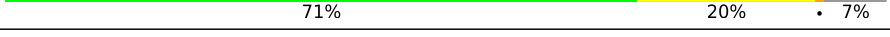
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	308	 73% 19% 7%
1	B	308	 81% 12% 7%
1	C	308	 79% 16% 5%
1	D	308	 71% 20% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9050 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 C-1-tetrahydrofolate synthase, cytoplasmic, N-terminally processed.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2136	1346	368	411	11			
1	B	286	Total	C	N	O	S	0	0	0
			2133	1347	365	410	11			
1	C	292	Total	C	N	O	S	0	0	0
			2186	1374	381	420	11			
1	D	285	Total	C	N	O	S	0	0	0
			2121	1337	366	407	11			

There are 36 discrepancies between the modelled and reference sequences:

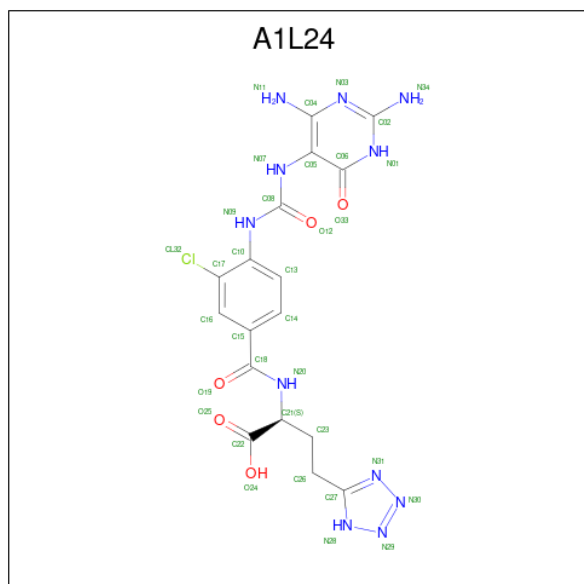
Chain	Residue	Modelled	Actual	Comment	Reference
A	134	ARG	LYS	variant	UNP P11586
A	302	LEU	-	expression tag	UNP P11586
A	303	GLU	-	expression tag	UNP P11586
A	304	HIS	-	expression tag	UNP P11586
A	305	HIS	-	expression tag	UNP P11586
A	306	HIS	-	expression tag	UNP P11586
A	307	HIS	-	expression tag	UNP P11586
A	308	HIS	-	expression tag	UNP P11586
A	309	HIS	-	expression tag	UNP P11586
B	134	ARG	LYS	variant	UNP P11586
B	302	LEU	-	expression tag	UNP P11586
B	303	GLU	-	expression tag	UNP P11586
B	304	HIS	-	expression tag	UNP P11586
B	305	HIS	-	expression tag	UNP P11586
B	306	HIS	-	expression tag	UNP P11586
B	307	HIS	-	expression tag	UNP P11586
B	308	HIS	-	expression tag	UNP P11586
B	309	HIS	-	expression tag	UNP P11586
C	134	ARG	LYS	variant	UNP P11586
C	302	LEU	-	expression tag	UNP P11586

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	303	GLU	-	expression tag	UNP P11586
C	304	HIS	-	expression tag	UNP P11586
C	305	HIS	-	expression tag	UNP P11586
C	306	HIS	-	expression tag	UNP P11586
C	307	HIS	-	expression tag	UNP P11586
C	308	HIS	-	expression tag	UNP P11586
C	309	HIS	-	expression tag	UNP P11586
D	134	ARG	LYS	variant	UNP P11586
D	302	LEU	-	expression tag	UNP P11586
D	303	GLU	-	expression tag	UNP P11586
D	304	HIS	-	expression tag	UNP P11586
D	305	HIS	-	expression tag	UNP P11586
D	306	HIS	-	expression tag	UNP P11586
D	307	HIS	-	expression tag	UNP P11586
D	308	HIS	-	expression tag	UNP P11586
D	309	HIS	-	expression tag	UNP P11586

- Molecule 2 is (2 {S})-2-[[4-[[2,4-bis(azanyl)-6-oxidanylidene-1 {H}-pyrimidin-5-yl]carbamoylamino]-3-chloranyl-phenyl]carbonylamino]-4-(1 {H}-1,2,3,4-tetrazol-5-yl)butanoic acid (CCD ID: A1L24) (formula: C₁₇H₁₈ClN₁₁O₅).



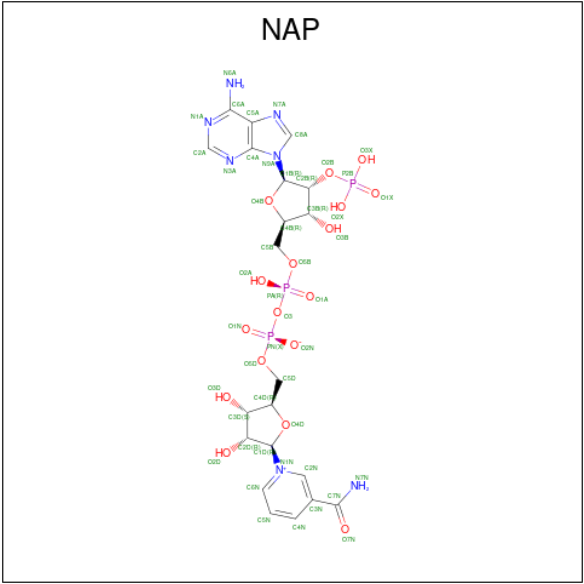
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			34	17	1	11	5		
2	B	1	Total	C	Cl	N	O	0	0
			34	17	1	11	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 34	C 17	Cl 1	N 11	O 5	0	0
2	D	1	Total 34	C 17	Cl 1	N 11	O 5	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

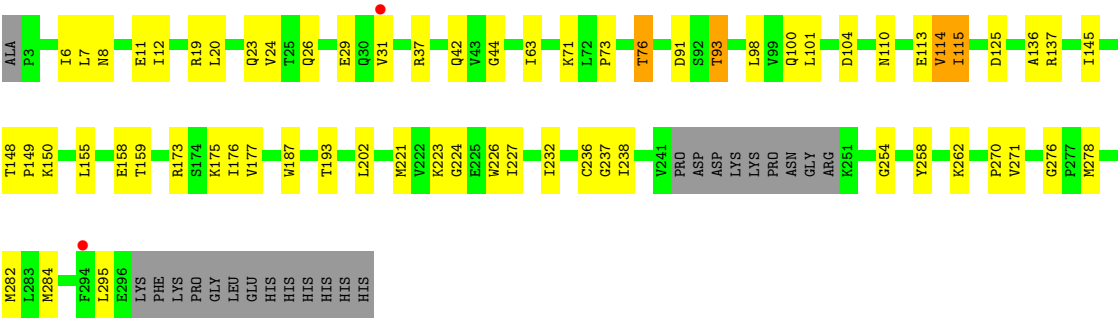
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	44	Total	O	0	0
			44	44		
4	C	40	Total	O	0	0
			40	40		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	22	Total	O	0	0
			22	22		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	65.08Å 201.47Å 240.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (30.00-2.50) 95.9 (30.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.213 , 0.264 0.213 , 0.264	Depositor DCC
R_{free} test set	2694 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9050	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: A1L24, NAP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/2168	0.67	0/2945
1	B	0.42	0/2166	0.62	1/2945 (0.0%)
1	C	0.39	0/2219	0.60	0/3015
1	D	0.41	0/2153	0.64	0/2928
All	All	0.41	0/8706	0.63	1/11833 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	ILE	N-CA-C	-5.15	107.81	112.96

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	2136	0	2173	48	0
1	B	2133	0	2162	25	0
1	C	2186	0	2217	35	0
1	D	2121	0	2145	42	0
2	A	34	0	0	2	0
2	B	34	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	34	0	0	2	0
2	D	34	0	0	1	0
3	A	48	0	25	3	0
3	B	48	0	25	2	0
3	C	48	0	25	2	0
3	D	48	0	25	3	0
4	A	40	0	0	0	0
4	B	44	0	0	0	0
4	C	40	0	0	0	0
4	D	22	0	0	0	0
All	All	9050	0	8797	145	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 8.

All (145) 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:A:101:LEU:HD12	1:A:176:ILE:HD11	1.53	0.90
1:B:236:CYS:HB3	3:B:402:NAP:H2N	1.56	0.88
1:A:72:LEU:HB3	1:A:76:THR:HG21	1.57	0.86
1:D:37:ARG:HD2	1:D:93:THR:HG23	1.60	0.82
1:D:238:ILE:HG12	3:D:402:NAP:H2N	1.63	0.79
1:C:12:ILE:HD13	1:C:158:GLU:HG3	1.67	0.75
1:C:44:GLY:HA3	1:C:104:ASP:HB3	1.70	0.74
1:A:82:MET:HE1	1:A:114:VAL:HA	1.71	0.73
1:A:282:MET:HA	1:A:282:MET:HE2	1.73	0.71
1:A:73:PRO:O	1:A:76:THR:HG23	1.91	0.70
1:B:6:ILE:HD11	1:B:258:TYR:OH	1.93	0.68
1:C:17:ARG:HG2	1:C:63:ILE:HD11	1.77	0.66
1:C:150:LYS:HE3	1:C:282:MET:HE3	1.77	0.66
1:A:172:GLY:HA2	3:A:402:NAP:H1B	1.78	0.66
1:A:288:VAL:O	1:A:292:LYS:HG3	1.95	0.65
1:D:63:ILE:HD12	1:D:284:MET:HG3	1.78	0.65
1:A:205:GLU:HA	1:A:208:LYS:HD2	1.78	0.65
1:A:254:GLY:HA3	1:A:271:VAL:HG21	1.79	0.64
1:D:237:GLY:O	1:D:238:ILE:HD13	1.99	0.63
1:D:31:VAL:HG21	1:D:295:LEU:HD21	1.80	0.62
1:B:236:CYS:O	3:B:402:NAP:H1D	2.00	0.61
1:C:43:VAL:HB	1:C:103:LEU:HD12	1.83	0.61
1:C:125:ASP:HB3	1:C:127:LEU:HG	1.81	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLY:HA3	1:A:104:ASP:HB3	1.84	0.60
1:C:137:ARG:HB3	1:D:175:LYS:HG2	1.84	0.60
1:D:6:ILE:HD11	1:D:262:LYS:HE3	1.82	0.60
1:D:125:ASP:OD2	2:D:401:A1L24:N34	2.36	0.59
1:C:229:PRO:HG3	1:C:264:ARG:HH21	1.68	0.58
1:A:10:LYS:HE2	1:A:273:GLY:HA3	1.85	0.58
1:B:46:ARG:HB2	1:B:49:SER:HB2	1.86	0.58
1:D:271:VAL:O	1:D:271:VAL:HG23	2.04	0.57
1:A:31:VAL:HG21	1:A:295:LEU:HD13	1.85	0.57
2:A:401:A1L24:CL32	3:A:402:NAP:C2N	2.91	0.56
1:B:101:LEU:O	2:B:401:A1L24:N11	2.40	0.55
1:B:262:LYS:HG3	1:B:268:ILE:HG21	1.88	0.55
1:B:120:PRO:HG3	1:B:130:ILE:HD12	1.87	0.54
1:A:137:ARG:HB3	1:B:175:LYS:HD3	1.90	0.54
1:D:271:VAL:O	1:D:271:VAL:CG2	2.54	0.54
1:C:187:TRP:CZ3	1:D:173:ARG:HD2	2.42	0.54
1:D:223:LYS:HA	1:D:223:LYS:HE3	1.90	0.54
1:D:136:ALA:O	1:D:137:ARG:HD3	2.08	0.53
1:D:150:LYS:HB3	1:D:282:MET:HG3	1.90	0.53
1:D:224:GLY:HA2	1:D:227:ILE:HD12	1.91	0.52
1:A:125:ASP:OD2	2:A:401:A1L24:N34	2.42	0.52
1:C:207:ASN:O	1:C:228:LYS:HB2	2.09	0.52
1:D:254:GLY:N	1:D:271:VAL:HG21	2.25	0.51
1:A:72:LEU:HD21	1:A:84:TYR:CE2	2.45	0.51
1:B:52:TYR:CE2	2:B:401:A1L24:CL32	3.00	0.51
1:D:42:GLN:OE1	1:D:71:LYS:HE2	2.09	0.51
1:C:40:ILE:HG12	1:C:98:LEU:HD11	1.93	0.51
1:C:229:PRO:HG3	1:C:264:ARG:NH2	2.25	0.51
1:D:258:TYR:CE2	1:D:270:PRO:HA	2.45	0.51
1:C:38:LEU:HD11	1:C:98:LEU:HD12	1.92	0.50
1:A:10:LYS:HE2	1:A:273:GLY:O	2.12	0.50
1:B:97:PHE:CE1	1:B:118:ILE:HG12	2.46	0.50
1:B:52:TYR:OH	1:B:238:ILE:HG21	2.10	0.50
1:A:196:HIS:CE1	1:A:198:LYS:HB2	2.46	0.50
1:C:42:GLN:HG2	1:C:71:LYS:HG3	1.94	0.49
1:B:125:ASP:HB3	1:B:127:LEU:HG	1.93	0.49
1:D:101:LEU:HD11	1:D:115:ILE:HD11	1.94	0.49
1:C:23:GLN:O	1:C:27:LEU:HD23	2.13	0.49
1:A:282:MET:HE1	1:A:285:GLN:OE1	2.13	0.48
1:A:63:ILE:HD13	1:A:284:MET:HG3	1.95	0.48
1:C:173:ARG:HD2	1:D:187:TRP:CZ3	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:HIS:HD2	1:A:294:PHE:CD1	2.32	0.48
1:B:56:LYS:HG2	1:B:280:VAL:HG13	1.96	0.48
1:C:149:PRO:HG2	1:C:180:PRO:HB2	1.96	0.48
1:C:175:LYS:HE3	1:D:137:ARG:HB3	1.95	0.48
1:C:145:ILE:HG22	1:C:150:LYS:HG3	1.97	0.47
1:A:187:TRP:CZ3	1:B:173:ARG:HD2	2.50	0.47
1:C:98:LEU:H	1:C:98:LEU:HD13	1.79	0.47
1:D:91:ASP:OD1	1:D:93:THR:HB	2.15	0.47
1:A:95:HIS:CD2	1:A:294:PHE:CD1	3.03	0.47
1:A:286:SER:O	1:A:289:GLU:HB2	2.15	0.47
1:B:153:LEU:HD22	1:B:184:LEU:HD22	1.95	0.47
1:A:173:ARG:HD2	1:B:187:TRP:CZ3	2.49	0.47
1:A:30:GLN:O	1:A:32:PRO:HD3	2.16	0.46
1:D:110:ASN:O	1:D:114:VAL:HG13	2.15	0.46
1:A:60:ALA:HB1	1:A:65:ILE:HB	1.98	0.46
1:A:37:ARG:HG2	1:A:66:LYS:HB2	1.98	0.46
1:B:125:ASP:OD2	2:B:401:A1L24:N34	2.49	0.46
1:B:227:ILE:O	1:B:264:ARG:NH1	2.49	0.46
1:A:82:MET:CE	1:A:114:VAL:HA	2.41	0.45
1:A:88:LEU:HA	1:A:88:LEU:HD23	1.72	0.45
1:D:73:PRO:O	1:D:76:THR:HB	2.17	0.45
1:D:110:ASN:HB3	1:D:113:GLU:HB2	1.98	0.45
1:C:150:LYS:HB3	1:C:282:MET:HG3	1.99	0.45
1:A:282:MET:HA	1:A:282:MET:CE	2.44	0.45
1:A:6:ILE:H	1:A:6:ILE:HD12	1.82	0.45
1:A:74:ARG:O	1:A:105:SER:HA	2.17	0.45
1:A:115:ILE:HD13	1:A:115:ILE:HA	1.80	0.44
2:C:401:A1L24:CL32	3:C:402:NAP:H2N	2.54	0.44
1:C:105:SER:HB3	1:C:107:ASN:O	2.18	0.44
1:C:38:LEU:HB2	1:C:287:THR:HG21	1.99	0.44
1:C:97:PHE:CZ	1:C:118:ILE:HG23	2.53	0.44
1:D:8:ASN:HB3	1:D:11:GLU:HB2	1.99	0.44
1:A:53:ILE:HG21	1:A:69:HIS:CE1	2.53	0.44
1:D:176:ILE:HG23	1:D:177:VAL:HG23	2.00	0.44
1:B:78:GLU:HB2	1:B:109:ILE:HG23	1.99	0.43
1:B:223:LYS:HA	1:B:223:LYS:HD2	1.66	0.43
1:C:16:ILE:HD11	1:C:278:MET:HE1	2.00	0.43
1:D:12:ILE:HD11	1:D:158:GLU:HG2	2.00	0.43
1:A:27:LEU:HD21	1:A:34:PHE:HE2	1.82	0.43
1:A:240:TYR:HA	1:A:251:LYS:O	2.19	0.43
1:D:26:GLN:O	1:D:29:GLU:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:CYS:O	3:D:402:NAP:H1D	2.18	0.43
1:A:59:ALA:O	1:A:63:ILE:HD12	2.19	0.43
2:C:401:A1L24:CL32	3:C:402:NAP:C2N	3.04	0.43
1:D:148:THR:HB	1:D:149:PRO:HD3	2.00	0.43
1:A:221:MET:HB3	1:A:221:MET:HE3	1.73	0.42
1:D:100:GLN:HG3	1:D:101:LEU:N	2.33	0.42
1:A:276:GLY:HA2	3:A:402:NAP:H72N	1.85	0.42
1:B:185:LEU:HA	1:B:185:LEU:HD23	1.85	0.42
1:A:10:LYS:CE	1:A:273:GLY:HA3	2.49	0.42
1:A:216:THR:HG21	1:A:221:MET:HE1	2.00	0.42
1:C:98:LEU:HD13	1:C:98:LEU:N	2.35	0.42
1:D:221:MET:HE3	1:D:221:MET:HB3	1.65	0.42
1:D:276:GLY:HA2	3:D:402:NAP:H72N	1.84	0.42
1:D:20:LEU:O	1:D:24:VAL:HG23	2.19	0.42
1:B:258:TYR:OH	1:B:262:LYS:HE3	2.20	0.42
1:C:168:ALA:HB1	1:C:185:LEU:HD13	2.01	0.42
1:D:44:GLY:HA3	1:D:104:ASP:HB3	2.00	0.42
1:B:12:ILE:CD1	1:B:158:GLU:HG2	2.50	0.42
1:C:34:PHE:CE1	1:C:295:LEU:HD21	2.55	0.42
1:A:92:SER:O	1:A:294:PHE:CE1	2.73	0.41
1:A:271:VAL:HA	1:A:272:PRO:HA	1.94	0.41
1:C:12:ILE:O	1:C:16:ILE:HG13	2.19	0.41
1:A:63:ILE:CD1	1:A:284:MET:HG3	2.51	0.41
1:D:19:ARG:HH11	1:D:23:GLN:NE2	2.18	0.41
1:A:27:LEU:CD2	1:A:34:PHE:HE2	2.34	0.41
1:A:278:MET:HE3	1:A:278:MET:HB3	1.66	0.41
1:C:53:ILE:HG21	1:C:69:HIS:CE1	2.55	0.41
1:C:65:ILE:HD11	1:C:288:VAL:HG23	2.03	0.41
1:C:146:PRO:HB2	1:C:149:PRO:HD2	2.03	0.41
1:D:159:THR:HG21	1:D:232:ILE:HD13	2.02	0.41
1:D:202:LEU:HD23	1:D:226:TRP:CZ3	2.56	0.41
1:B:37:ARG:NH1	1:B:37:ARG:HB3	2.36	0.41
1:C:98:LEU:C	1:C:98:LEU:HD22	2.47	0.40
1:D:155:LEU:HG	1:D:278:MET:HG3	2.02	0.40
1:A:10:LYS:HE2	1:A:273:GLY:CA	2.51	0.40
1:B:42:GLN:OE1	1:B:71:LYS:HE2	2.21	0.40
1:C:192:VAL:O	1:D:193:THR:HA	2.22	0.40
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.88	0.40
1:D:7:LEU:O	1:D:270:PRO:HD2	2.21	0.40
1:C:240:TYR:CE1	1:C:252:VAL:HG22	2.56	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	281/308 (91%)	272 (97%)	9 (3%)	0	100	100
1	B	282/308 (92%)	277 (98%)	5 (2%)	0	100	100
1	C	288/308 (94%)	280 (97%)	8 (3%)	0	100	100
1	D	281/308 (91%)	271 (96%)	10 (4%)	0	100	100
All	All	1132/1232 (92%)	1100 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	234/260 (90%)	231 (99%)	3 (1%)	61	82
1	B	232/260 (89%)	231 (100%)	1 (0%)	84	93
1	C	238/260 (92%)	236 (99%)	2 (1%)	73	88
1	D	230/260 (88%)	224 (97%)	6 (3%)	40	68
All	All	934/1040 (90%)	922 (99%)	12 (1%)	61	82

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	LEU
1	A	125	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	154	GLU
1	B	98	LEU
1	C	98	LEU
1	C	266	SER
1	D	76	THR
1	D	93	THR
1	D	98	LEU
1	D	114	VAL
1	D	115	ILE
1	D	145	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	69	HIS
1	B	201	HIS
1	B	207	ASN
1	C	45	ASN
1	C	207	ASN
1	D	54	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	A1L24	C	401	-	35,36,36	2.04	10 (28%)	46,50,50	1.34	8 (17%)
3	NAP	A	402	-	50,52,52	0.55	0	71,80,80	0.83	2 (2%)
2	A1L24	A	401	-	35,36,36	2.06	10 (28%)	46,50,50	1.16	5 (10%)
2	A1L24	B	401	-	35,36,36	2.07	11 (31%)	46,50,50	1.34	10 (21%)
3	NAP	D	402	-	50,52,52	0.55	0	71,80,80	0.78	2 (2%)
3	NAP	C	402	-	50,52,52	0.55	0	71,80,80	0.88	2 (2%)
2	A1L24	D	401	-	35,36,36	2.00	10 (28%)	46,50,50	1.38	6 (13%)
3	NAP	B	402	-	50,52,52	0.56	0	71,80,80	0.91	3 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1L24	C	401	-	-	0/25/25/25	0/3/3/3
3	NAP	A	402	-	-	7/35/67/67	0/5/5/5
2	A1L24	A	401	-	-	2/25/25/25	0/3/3/3
2	A1L24	B	401	-	-	1/25/25/25	0/3/3/3
3	NAP	D	402	-	-	13/35/67/67	0/5/5/5
3	NAP	C	402	-	-	5/35/67/67	0/5/5/5
2	A1L24	D	401	-	-	2/25/25/25	0/3/3/3
3	NAP	B	402	-	-	11/35/67/67	0/5/5/5

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	A1L24	C02-N34	5.21	1.46	1.34
2	C	401	A1L24	C02-N34	5.19	1.46	1.34
2	B	401	A1L24	C02-N34	4.98	1.45	1.34
2	D	401	A1L24	C02-N34	4.96	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	A1L24	C18-N20	4.88	1.45	1.34
2	C	401	A1L24	C04-N11	4.84	1.46	1.34
2	A	401	A1L24	C04-N11	4.67	1.46	1.34
2	D	401	A1L24	C04-N11	4.67	1.46	1.34
2	C	401	A1L24	C18-N20	4.62	1.44	1.34
2	A	401	A1L24	C18-N20	4.61	1.44	1.34
2	D	401	A1L24	C18-N20	4.47	1.44	1.34
2	B	401	A1L24	C04-N11	4.34	1.45	1.34
2	B	401	A1L24	C06-N01	-3.87	1.31	1.38
2	D	401	A1L24	C06-N01	-3.51	1.32	1.38
2	A	401	A1L24	C08-N09	3.32	1.44	1.37
2	C	401	A1L24	C06-N01	-3.32	1.32	1.38
2	C	401	A1L24	C08-N09	3.28	1.44	1.37
2	B	401	A1L24	C08-N09	3.16	1.44	1.37
2	A	401	A1L24	C06-N01	-3.14	1.33	1.38
2	D	401	A1L24	C08-N09	2.96	1.44	1.37
2	B	401	A1L24	O33-C06	-2.39	1.19	1.23
2	D	401	A1L24	C17-CL32	2.36	1.79	1.73
2	A	401	A1L24	C17-CL32	2.36	1.79	1.73
2	C	401	A1L24	C08-N07	2.35	1.44	1.39
2	A	401	A1L24	C08-N07	2.34	1.44	1.39
2	B	401	A1L24	C17-CL32	2.33	1.79	1.73
2	C	401	A1L24	O12-C08	-2.33	1.18	1.23
2	D	401	A1L24	C02-N01	-2.32	1.32	1.37
2	B	401	A1L24	C02-N01	-2.28	1.32	1.37
2	B	401	A1L24	C08-N07	2.22	1.44	1.39
2	D	401	A1L24	C26-C27	2.20	1.53	1.49
2	B	401	A1L24	C27-N28	2.15	1.37	1.33
2	D	401	A1L24	O12-C08	-2.15	1.18	1.23
2	B	401	A1L24	C26-C27	2.14	1.53	1.49
2	A	401	A1L24	C26-C27	2.12	1.53	1.49
2	A	401	A1L24	O12-C08	-2.11	1.18	1.23
2	C	401	A1L24	C17-CL32	2.08	1.78	1.73
2	C	401	A1L24	C10-N09	2.04	1.45	1.41
2	A	401	A1L24	C27-N28	2.04	1.37	1.33
2	C	401	A1L24	C02-N01	-2.03	1.32	1.37
2	D	401	A1L24	O19-C18	-2.03	1.18	1.23

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	NAP	P2B-O2B-C2B	-5.08	109.87	123.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	NAP	P2B-O2B-C2B	-4.65	111.00	123.43
3	A	402	NAP	P2B-O2B-C2B	-4.26	112.05	123.43
3	B	402	NAP	C6N-N1N-C2N	-4.16	118.34	121.88
3	B	402	NAP	P2B-O2B-C2B	-4.13	112.40	123.43
2	D	401	A1L24	N11-C04-N03	3.15	122.61	116.23
3	A	402	NAP	C6N-N1N-C2N	-3.08	119.26	121.88
2	C	401	A1L24	N11-C04-N03	2.98	122.25	116.23
3	D	402	NAP	C6N-N1N-C2N	-2.89	119.42	121.88
2	D	401	A1L24	C02-N03-C04	2.87	119.74	113.79
2	B	401	A1L24	O33-C06-C05	-2.85	120.39	127.26
3	C	402	NAP	C6N-N1N-C2N	-2.80	119.50	121.88
2	C	401	A1L24	C02-N03-C04	2.76	119.50	113.79
2	A	401	A1L24	C02-N03-C04	2.74	119.47	113.79
2	A	401	A1L24	N11-C04-N03	2.69	121.67	116.23
3	B	402	NAP	C5N-C4N-C3N	-2.55	117.86	120.36
2	B	401	A1L24	C16-C17-CL32	2.53	122.60	118.45
2	B	401	A1L24	C10-C17-CL32	-2.52	116.79	119.52
2	C	401	A1L24	C23-C21-N20	-2.50	105.97	110.91
2	D	401	A1L24	C23-C21-N20	-2.48	105.99	110.91
2	D	401	A1L24	C16-C17-C10	-2.48	119.80	121.77
2	B	401	A1L24	C06-C05-N07	-2.47	114.22	118.45
2	B	401	A1L24	C02-N03-C04	2.46	118.88	113.79
2	B	401	A1L24	O24-C22-C21	2.40	121.63	113.51
2	A	401	A1L24	C23-C21-N20	-2.38	106.20	110.91
2	C	401	A1L24	C06-C05-N07	2.34	122.46	118.45
2	B	401	A1L24	C05-C06-N01	2.28	118.40	112.13
2	A	401	A1L24	O33-C06-C05	-2.24	121.85	127.26
2	D	401	A1L24	C13-C10-C17	2.17	120.79	117.89
2	C	401	A1L24	C21-N20-C18	-2.16	116.38	121.56
2	B	401	A1L24	N11-C04-N03	2.16	120.61	116.23
2	B	401	A1L24	C02-N01-C06	-2.14	121.22	125.11
2	B	401	A1L24	O24-C22-O25	-2.13	119.25	124.08
2	C	401	A1L24	C16-C17-C10	-2.09	120.11	121.77
2	C	401	A1L24	N09-C08-N07	2.08	118.72	114.22
2	A	401	A1L24	C02-N01-C06	-2.06	121.37	125.11
2	D	401	A1L24	C02-N01-C06	-2.04	121.42	125.11
2	C	401	A1L24	C23-C26-C27	-2.01	106.90	114.38

There are no chirality outliers.

All (41) torsion outliers are listed below:

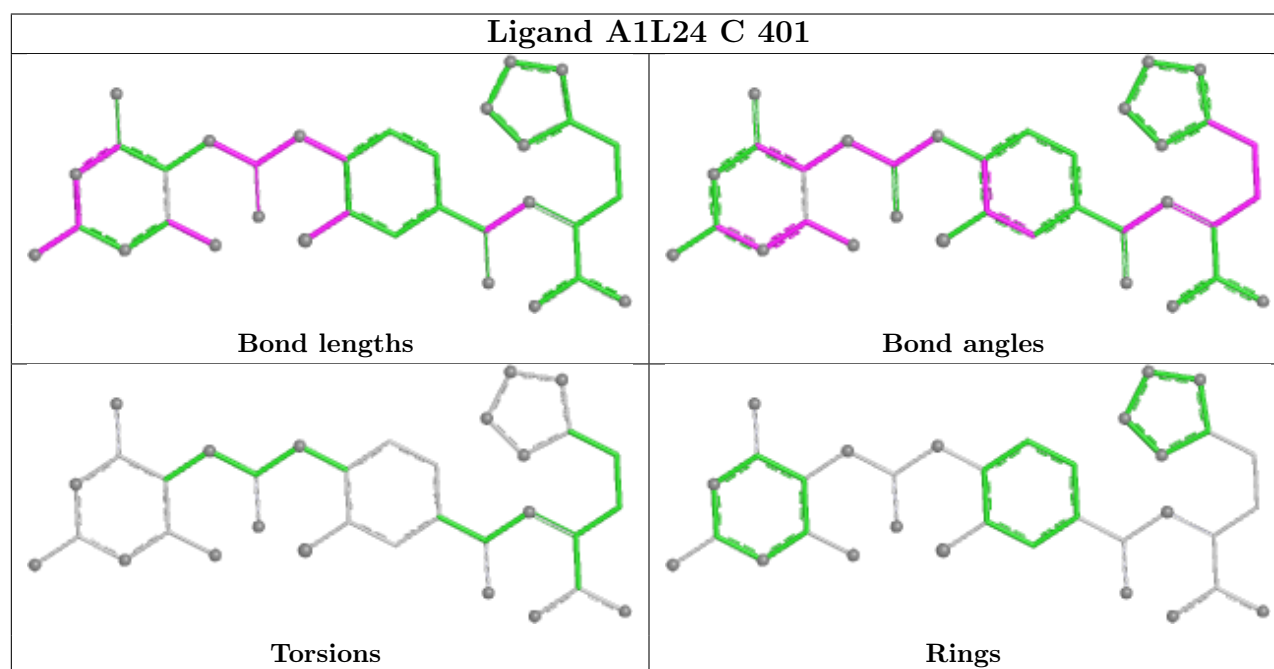
Mol	Chain	Res	Type	Atoms
3	A	402	NAP	C5B-O5B-PA-O2A
3	B	402	NAP	C5B-O5B-PA-O2A
3	B	402	NAP	O4D-C1D-N1N-C2N
3	B	402	NAP	O4D-C1D-N1N-C6N
3	B	402	NAP	C2D-C1D-N1N-C2N
3	B	402	NAP	C2D-C1D-N1N-C6N
3	C	402	NAP	C2N-C3N-C7N-O7N
3	C	402	NAP	C2N-C3N-C7N-N7N
3	D	402	NAP	C5B-O5B-PA-O1A
3	D	402	NAP	C5B-O5B-PA-O2A
3	D	402	NAP	C5B-O5B-PA-O3
3	D	402	NAP	O4B-C4B-C5B-O5B
3	C	402	NAP	C4N-C3N-C7N-N7N
3	C	402	NAP	C4N-C3N-C7N-O7N
3	A	402	NAP	C3B-C2B-O2B-P2B
3	D	402	NAP	C3B-C4B-C5B-O5B
2	B	401	A1L24	C21-C23-C26-C27
3	A	402	NAP	C1B-C2B-O2B-P2B
2	A	401	A1L24	N20-C21-C23-C26
3	D	402	NAP	C1B-C2B-O2B-P2B
3	D	402	NAP	C2N-C3N-C7N-N7N
3	D	402	NAP	C2N-C3N-C7N-O7N
3	A	402	NAP	PN-O3-PA-O5B
3	B	402	NAP	PN-O3-PA-O5B
3	D	402	NAP	PN-O3-PA-O5B
3	D	402	NAP	C3B-C2B-O2B-P2B
3	D	402	NAP	C4N-C3N-C7N-N7N
3	A	402	NAP	C5B-O5B-PA-O1A
3	A	402	NAP	C5B-O5B-PA-O3
3	B	402	NAP	C5B-O5B-PA-O1A
3	B	402	NAP	C5B-O5B-PA-O3
2	D	401	A1L24	C21-C23-C26-C27
3	D	402	NAP	C4N-C3N-C7N-O7N
2	A	401	A1L24	C22-C21-C23-C26
3	B	402	NAP	C1B-C2B-O2B-P2B
3	B	402	NAP	C2B-O2B-P2B-O1X
3	B	402	NAP	C3B-C2B-O2B-P2B
3	C	402	NAP	O4B-C4B-C5B-O5B
2	D	401	A1L24	N20-C21-C23-C26
3	D	402	NAP	C2B-O2B-P2B-O1X
3	A	402	NAP	PN-O3-PA-O2A

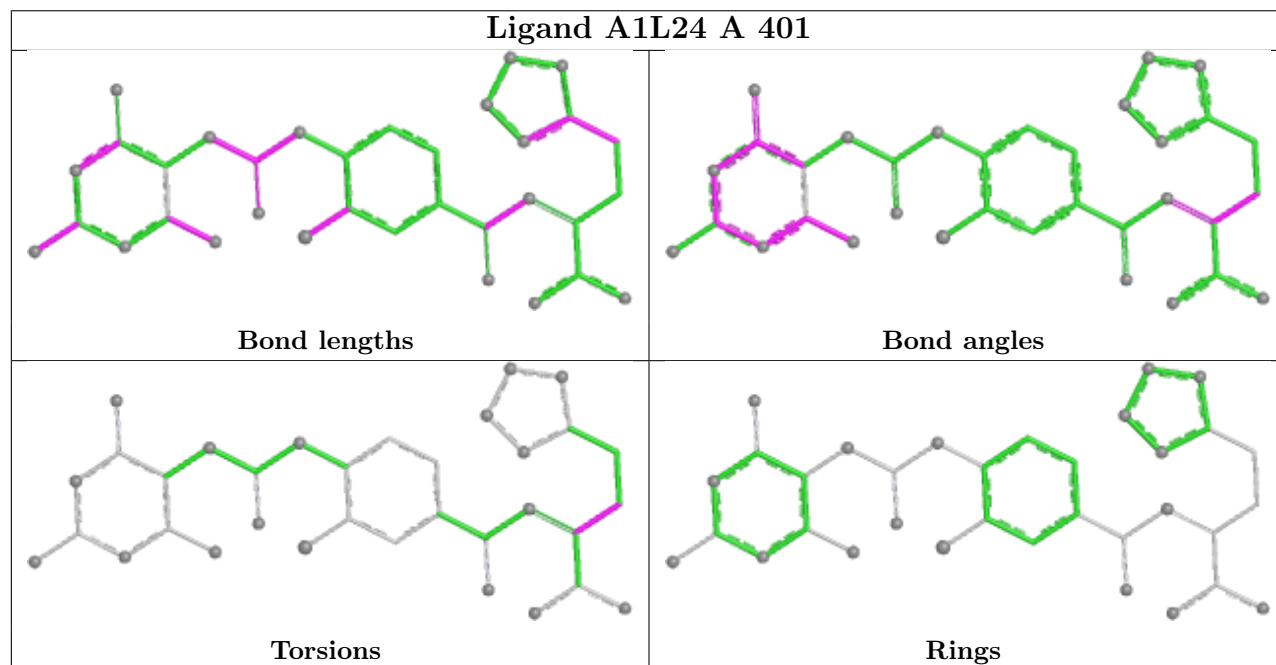
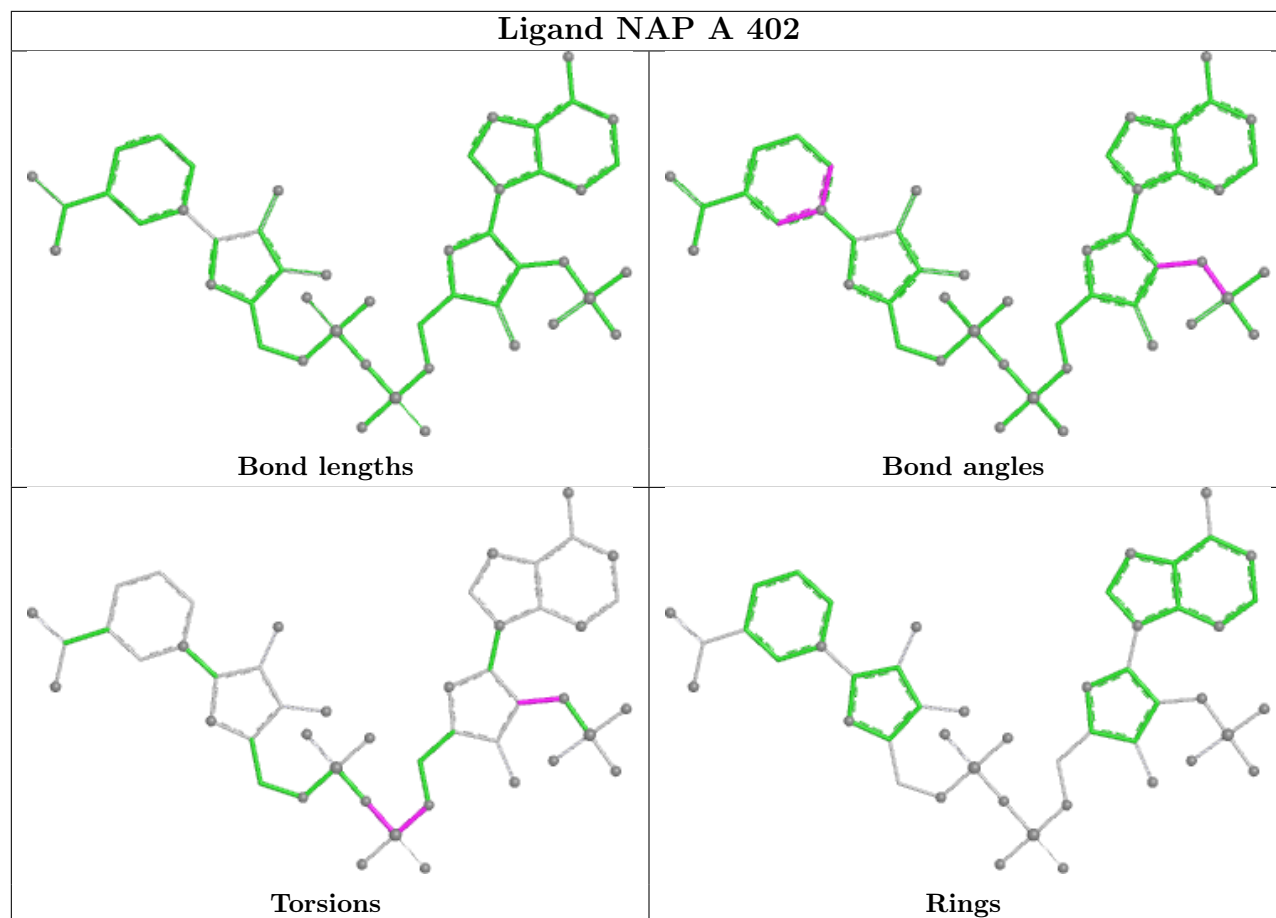
There are no ring outliers.

8 monomers are involved in 15 short contacts:

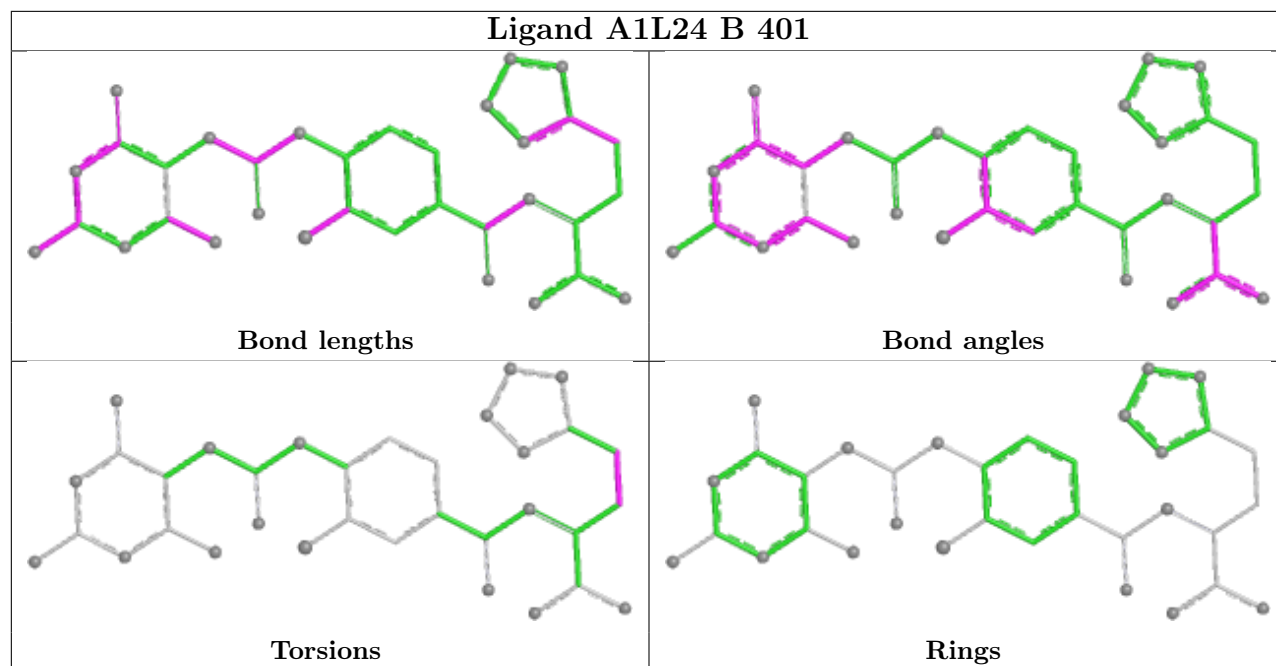
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	A1L24	2	0
3	A	402	NAP	3	0
2	A	401	A1L24	2	0
2	B	401	A1L24	3	0
3	D	402	NAP	3	0
3	C	402	NAP	2	0
2	D	401	A1L24	1	0
3	B	402	NAP	2	0

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

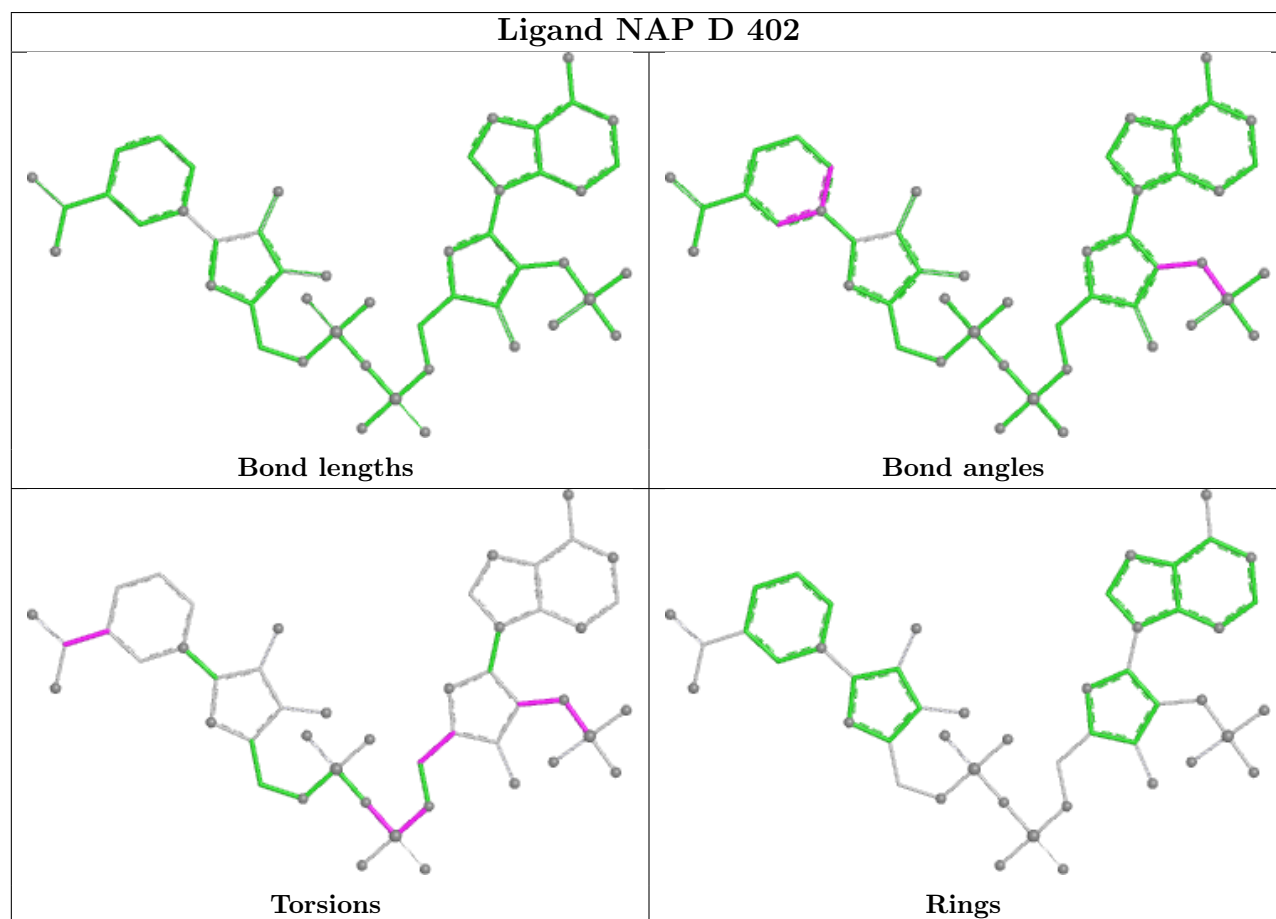


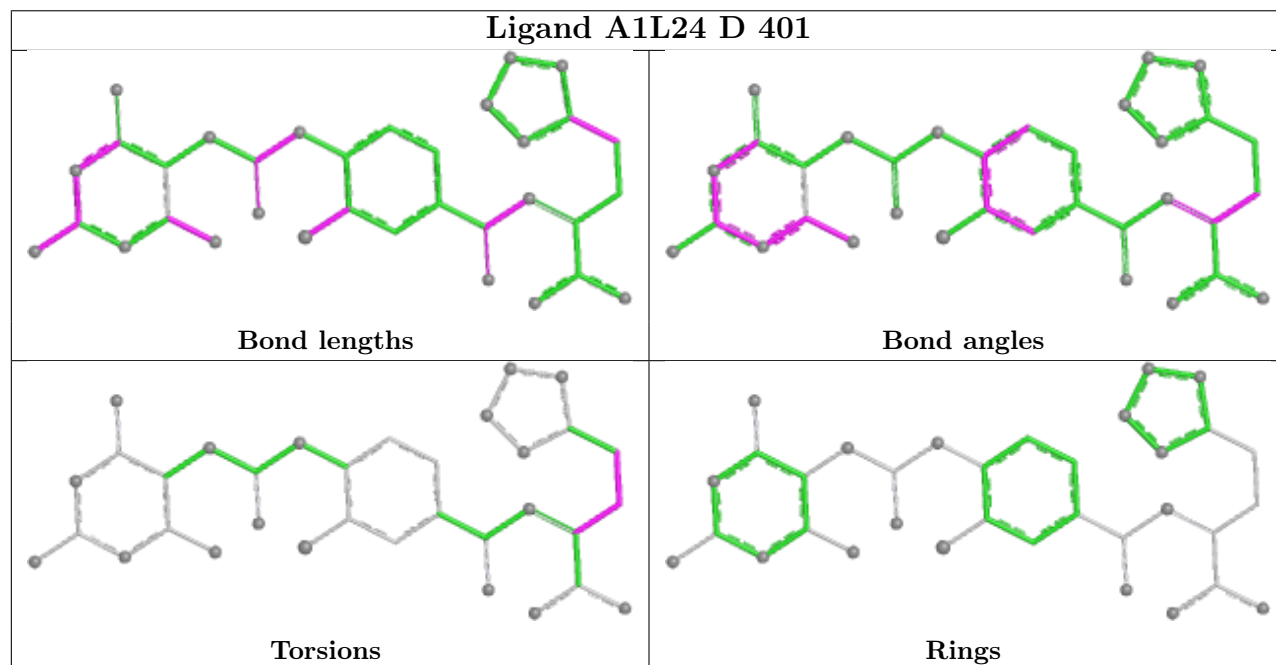
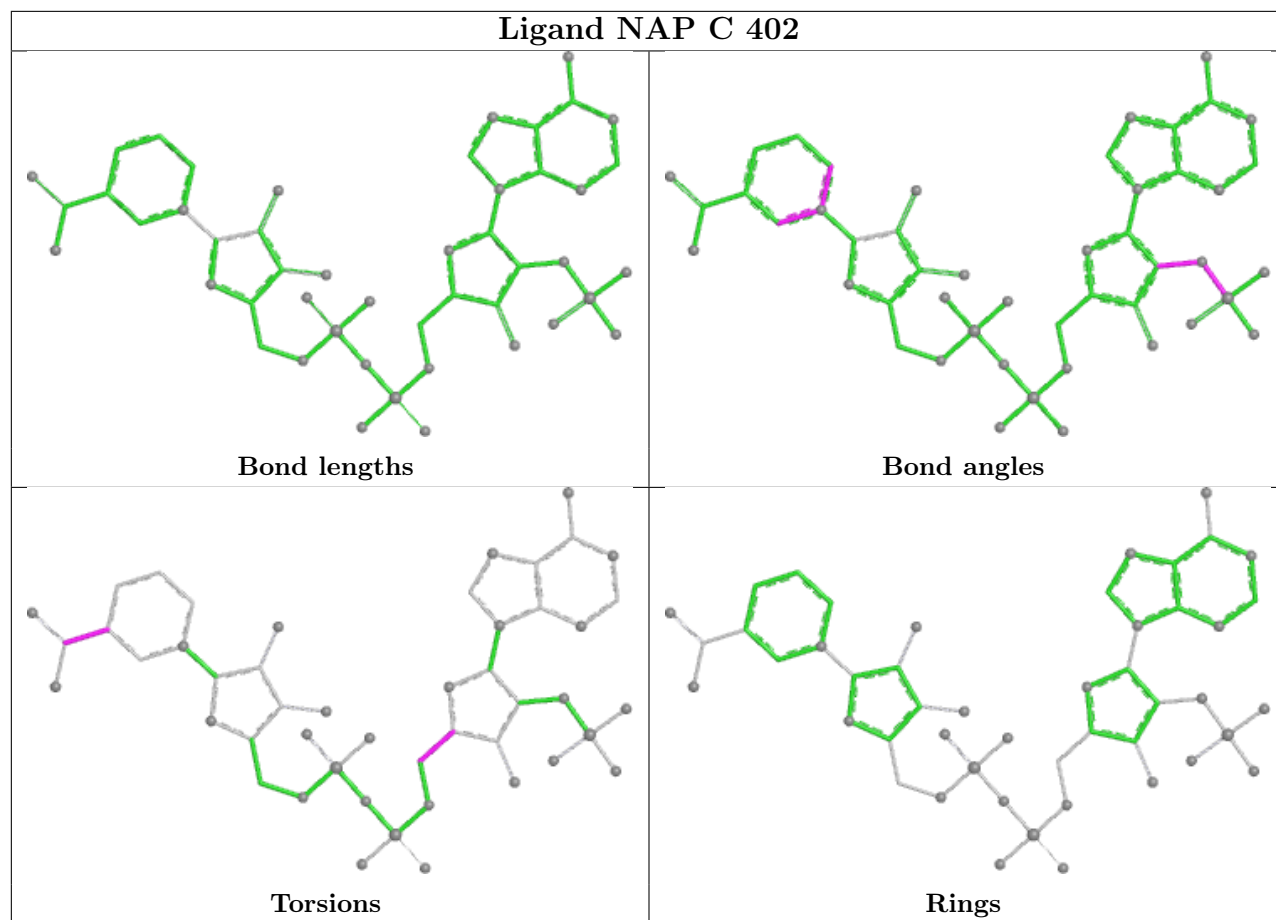


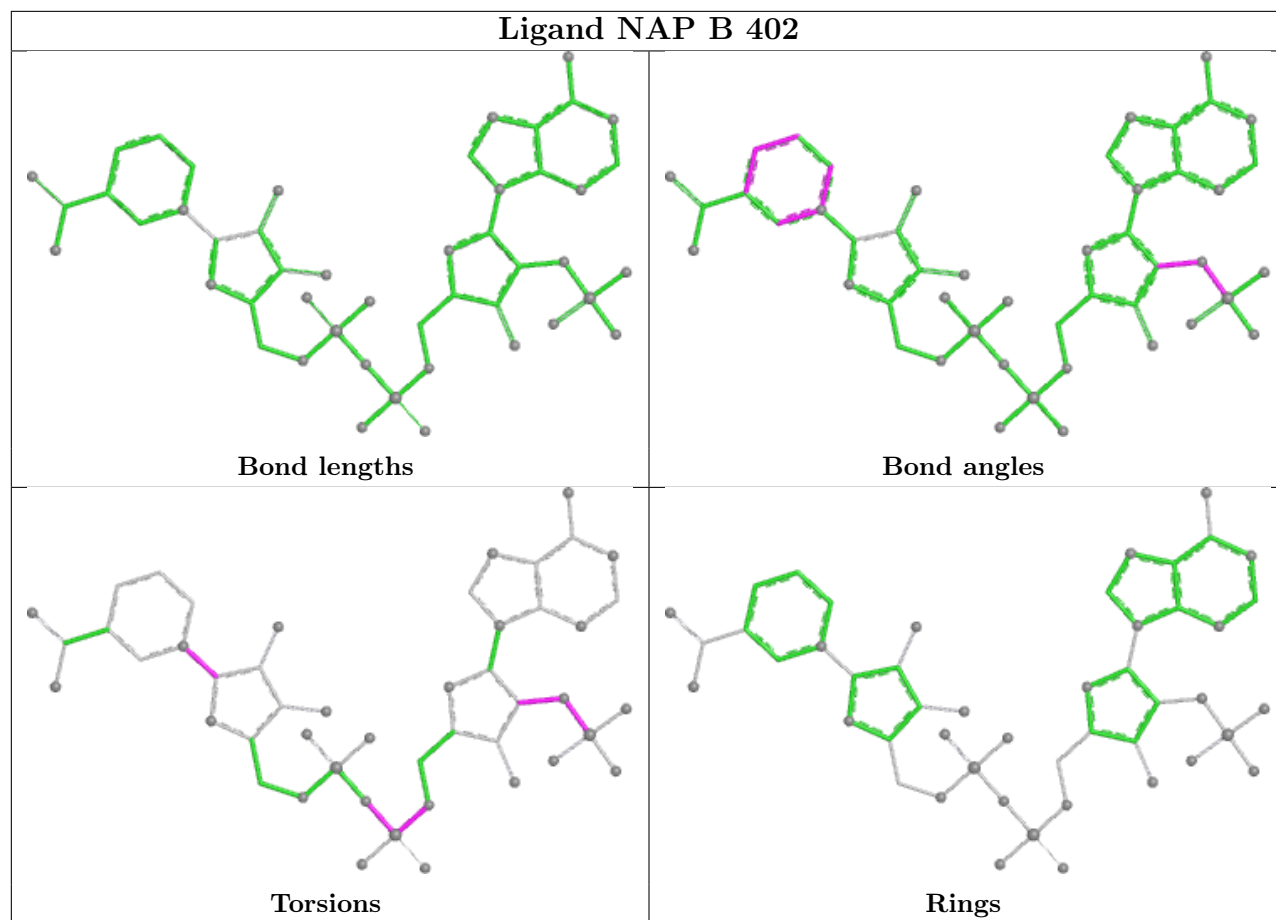
Ligand A1L24 B 401



Ligand NAP D 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	285/308 (92%)	-0.12	1 (0%) 88 86	24, 40, 60, 69	0
1	B	286/308 (92%)	-0.20	3 (1%) 79 76	27, 40, 59, 83	0
1	C	292/308 (94%)	-0.10	3 (1%) 79 76	24, 42, 64, 82	0
1	D	285/308 (92%)	0.33	2 (0%) 84 81	33, 52, 70, 91	0
All	All	1148/1232 (93%)	-0.03	9 (0%) 82 80	24, 43, 65, 91	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	294	PHE	3.6
1	C	249	GLY	3.2
1	C	2	ALA	2.6
1	B	296	GLU	2.5
1	B	31	VAL	2.5
1	D	31	VAL	2.5
1	A	142	ASP	2.2
1	C	32	PRO	2.1
1	B	3	PRO	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](#)

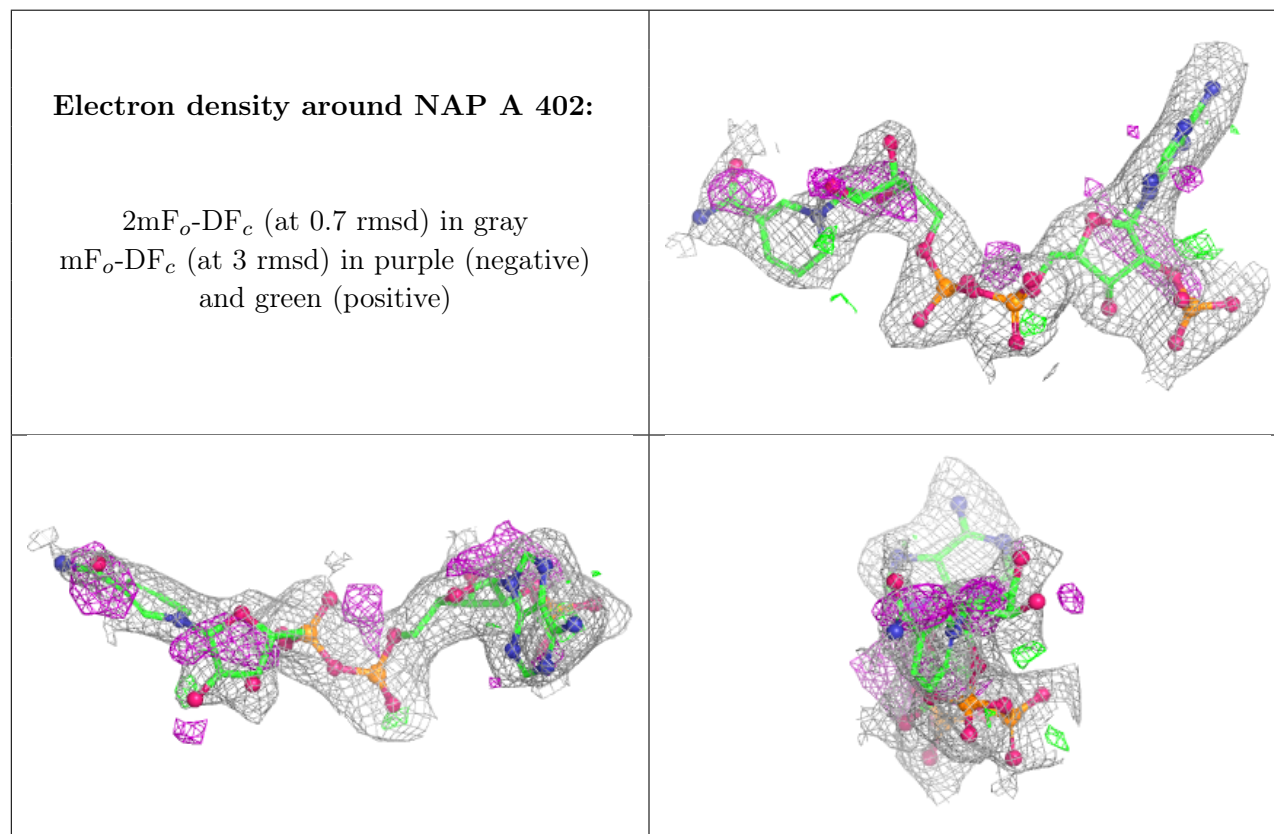
There are no oligosaccharides in this entry.

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.

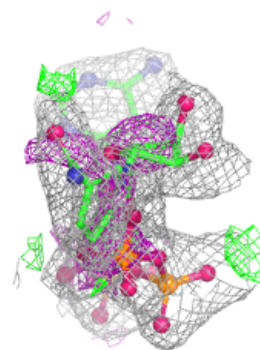
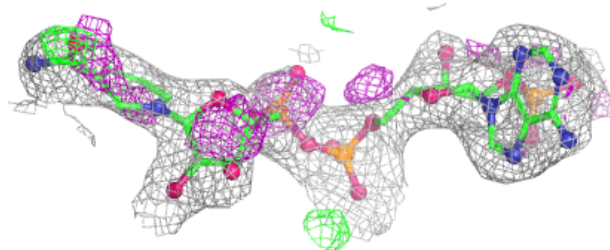
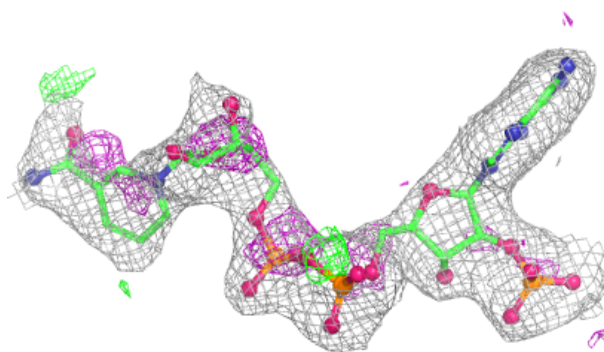
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	A	402	48/48	0.90	0.13	27,47,59,62	0
3	NAP	C	402	48/48	0.90	0.12	34,48,60,75	0
3	NAP	B	402	48/48	0.91	0.14	21,40,56,64	48
3	NAP	D	402	48/48	0.91	0.12	44,63,73,75	0
2	A1L24	D	401	34/34	0.92	0.09	41,58,76,76	0
2	A1L24	A	401	34/34	0.94	0.09	32,43,73,76	0
2	A1L24	B	401	34/34	0.95	0.07	30,41,58,61	0
2	A1L24	C	401	34/34	0.96	0.07	34,46,52,58	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

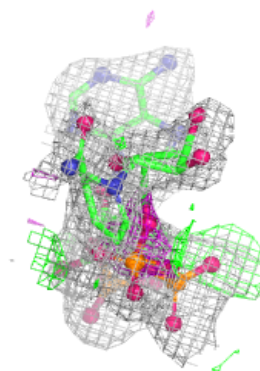
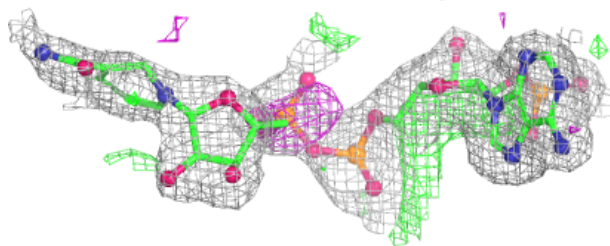
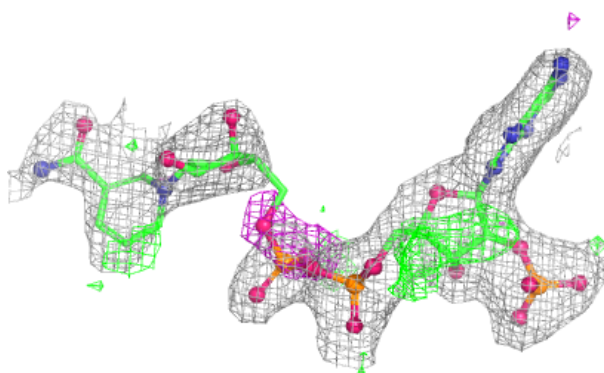


Electron density around NAP C 402:

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

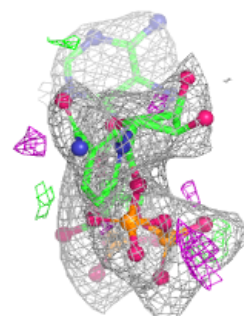
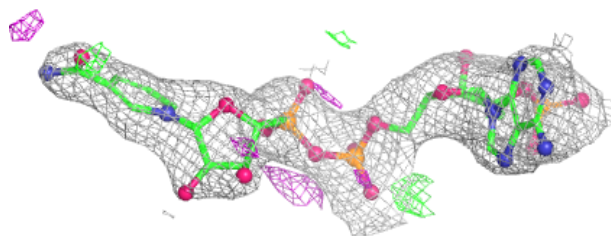
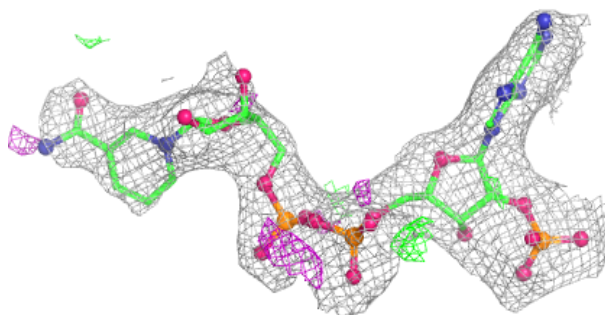
**Electron density around NAP B 402:**

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

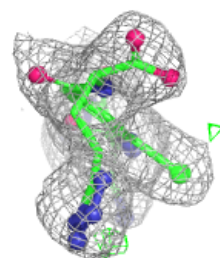
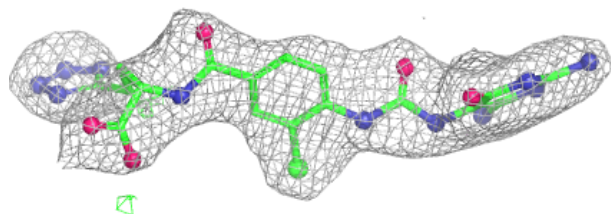
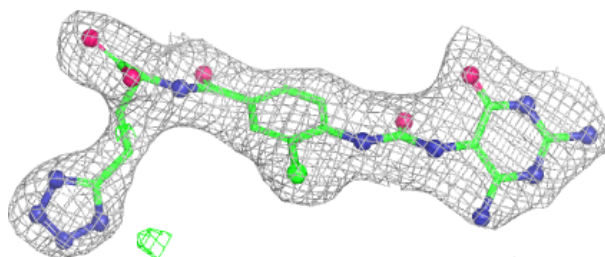


Electron density around NAP D 402:

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

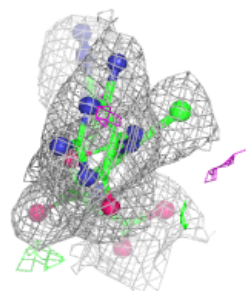
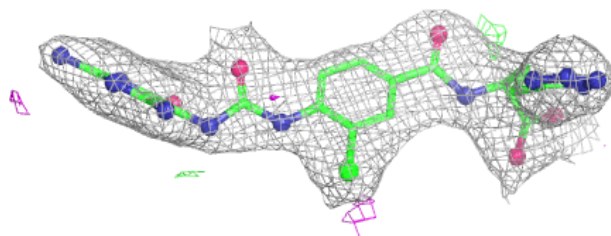
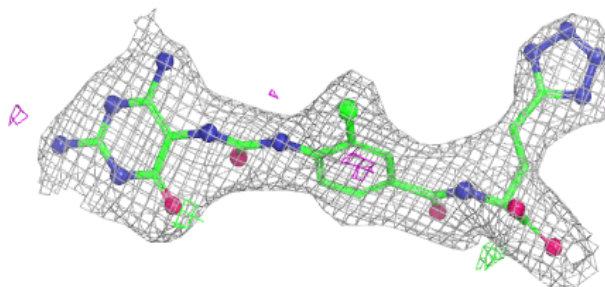
**Electron density around A1L24 D 401:**

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

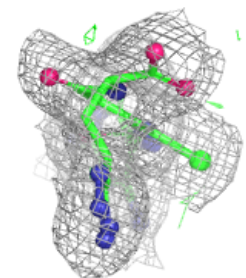
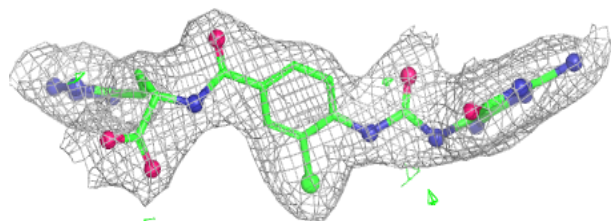
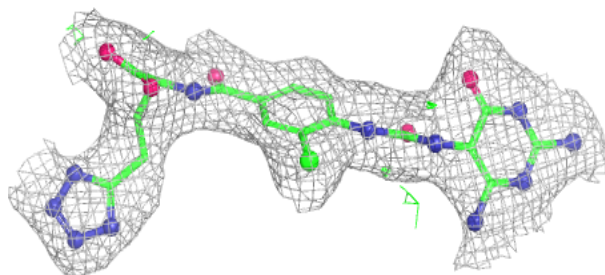


Electron density around A1L24 A 401:

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

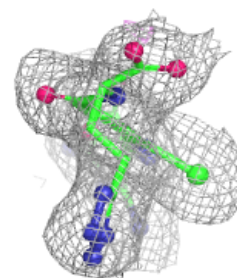
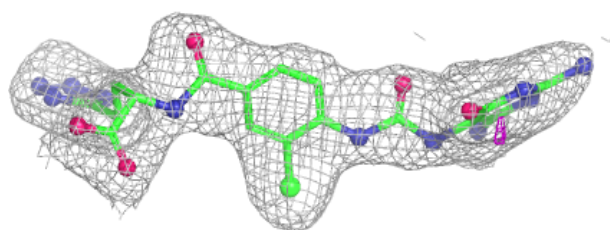
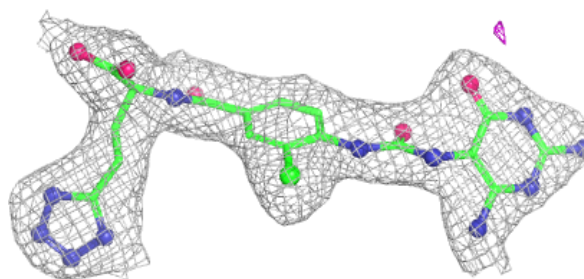
**Electron density around A1L24 B 401:**

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



Electron density around A1L24 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.