



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:05 PM UTC

PDB ID : 9ITD / pdb_00009itd
Title : Human MTHFD1 in complex with compound 16a
Authors : Lee, L.C.; Wu, S.Y.
Deposited on : 2024-07-19
Resolution : 2.28 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

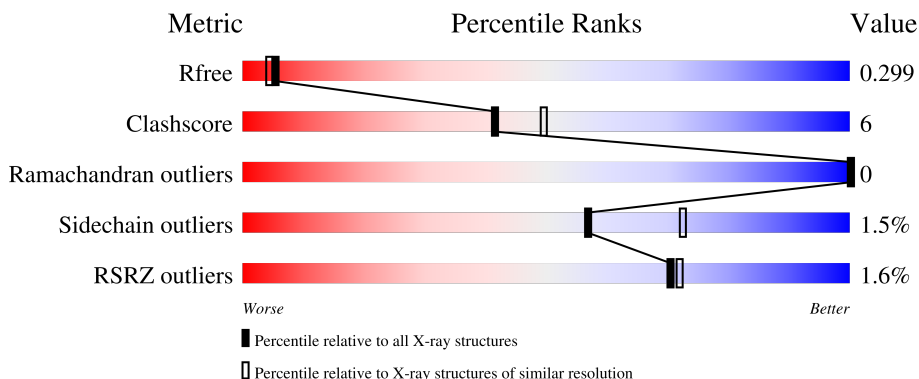
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	 78% 15% 7%
1	B	308	 3% 77% 16% 7%
1	C	308	 80% 15% 5%
1	D	308	 77% 15% 7%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9180 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
			Total	C	N	O	S			
1	A	286	2152	1354	372	415	11	0	0	0
1	B	286	2152	1354	372	415	11	0	0	0
1	C	294	2216	1391	386	428	11	0	0	0
1	D	286	2156	1356	372	417	11	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

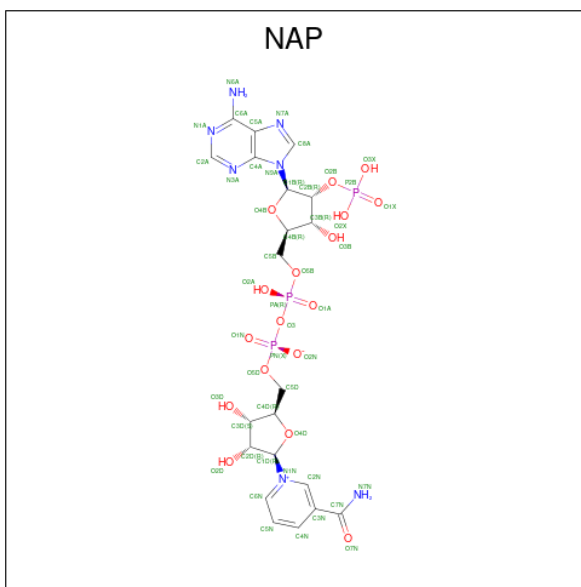
Chain	Residue	Modelled	Actual	Comment	Reference
A	134	ARG	LYS	variant	UNP P11586
A	302	LEU	-	expression tag	UNP P11586
A	303	GLU	-	expression tag	UNP P11586
A	304	HIS	-	expression tag	UNP P11586
A	305	HIS	-	expression tag	UNP P11586
A	306	HIS	-	expression tag	UNP P11586
A	307	HIS	-	expression tag	UNP 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 NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



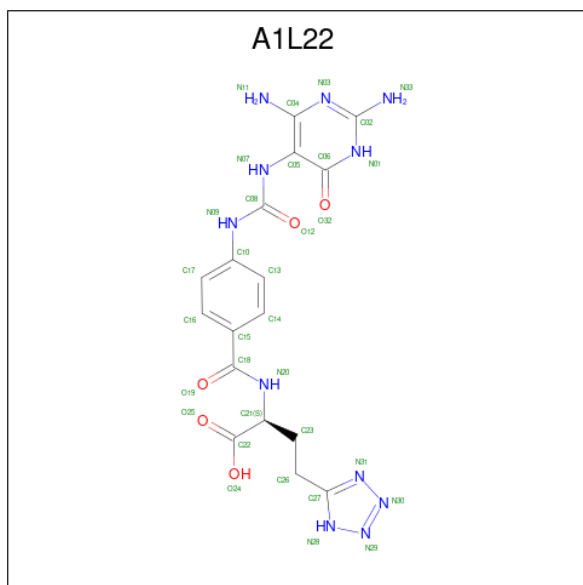
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is (2 {S})-2-[[4-[[2,4-bis(azanyl)-6-oxidanylidene-1 {H}-pyrimidin-5-yl]carbamoylamino]phenyl]carbonylamino]-4-(1 {H}-1,2,3,4-tetrazol-5-yl)butanoic acid (CCD ID: A1L22) (formula: C₁₇H₁₉N₁₁O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	33	17	11	5	0	0
3	B	1	33	17	11	5	0	0
3	C	1	33	17	11	5	0	0
3	D	1	33	17	11	5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	40	Total 40 O	0	0
4	B	56	Total 56 O	0	0
4	C	42	Total 42 O	0	0

Continued on next page...

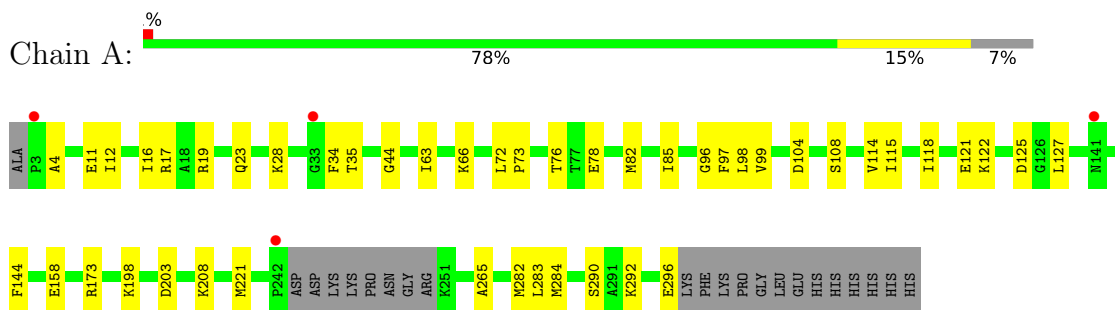
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	42	Total	O	0	0
			42	42		

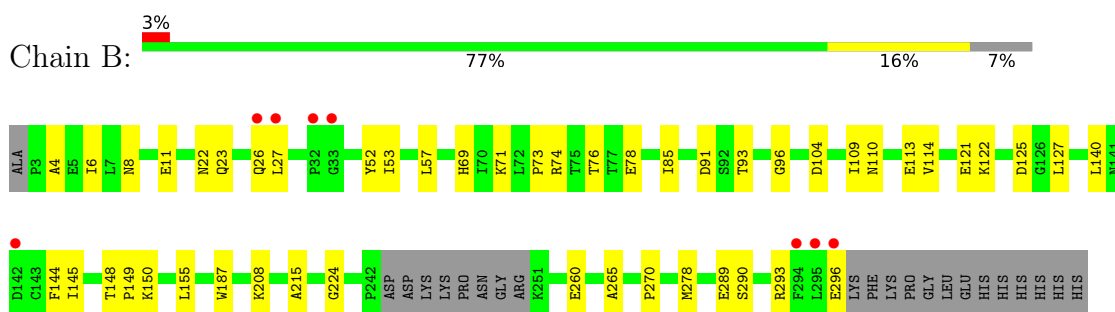
3 Residue-property plots [i](#)

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.

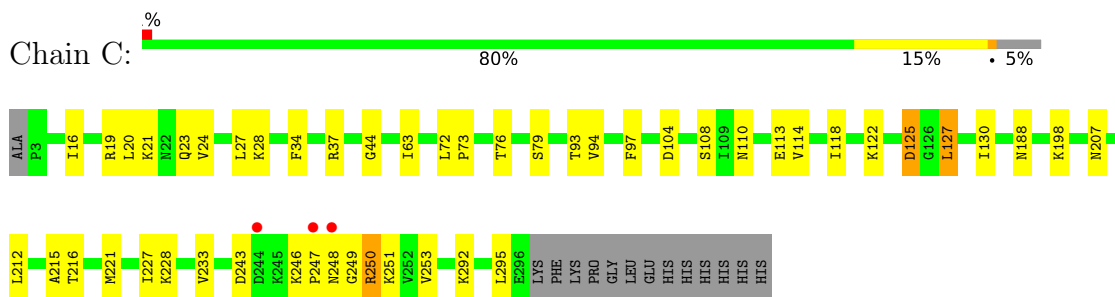
- Molecule 1: C-1-tetrahydrofolate synthase, cytoplasmic, N-terminally processed



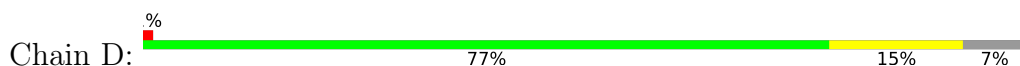
- Molecule 1: C-1-tetrahydrofolate synthase, cytoplasmic, N-terminally processed

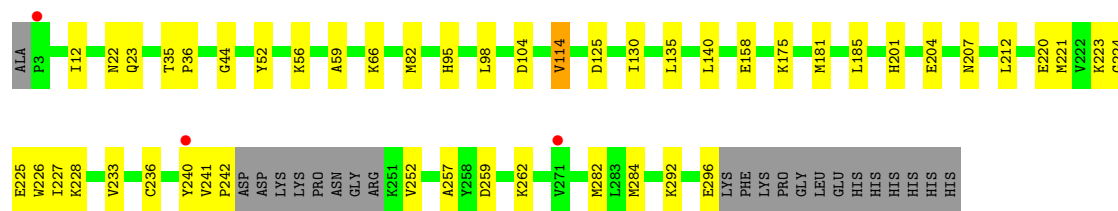


- Molecule 1: C-1-tetrahydrofolate synthase, cytoplasmic, N-terminally processed



- Molecule 1: C-1-tetrahydrofolate synthase, cytoplasmic, N-terminally processed





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	65.30Å 200.34Å 239.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.21 – 2.28 26.21 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.8 (26.21-2.28) 99.2 (26.21-2.28)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.26Å)	Xtrriage
Refinement program	PHENIX 1.21.1_5286_000	Depositor
R, R_{free}	0.237 , 0.299 0.237 , 0.299	Depositor DCC
R_{free} test set	3604 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtrriage
Anisotropy	0.244	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9180	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: NAP, A1L22

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	0.41	0/2185	0.62	2/2969 (0.1%)
1	B	0.40	0/2185	0.59	0/2969
1	C	0.44	1/2251 (0.0%)	0.64	1/3058 (0.0%)
1	D	0.37	1/2189 (0.0%)	0.56	0/2974
All	All	0.41	2/8810 (0.0%)	0.60	3/11970 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	22	ASN	CG-OD1	5.33	1.33	1.23
1	C	227	ILE	C-O	-5.06	1.18	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	188	ASN	N-CA-C	-8.74	102.75	112.72
1	A	203	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	198	LYS	N-CA-C	-5.34	106.54	113.16

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	2152	0	2188	28	0
1	B	2152	0	2188	31	0
1	C	2216	0	2252	29	0
1	D	2156	0	2192	28	0
2	A	48	0	25	1	0
2	B	48	0	25	2	0
2	C	48	0	25	1	0
2	D	48	0	25	1	0
3	A	33	0	0	2	0
3	B	33	0	0	0	0
3	C	33	0	0	0	0
3	D	33	0	0	0	0
4	A	40	0	0	0	0
4	B	56	0	0	0	0
4	C	42	0	0	0	0
4	D	42	0	0	0	0
All	All	9180	0	8920	114	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 6.

All (114) 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:73:PRO:HG2	1:B:76:THR:HG23	1.48	0.93
1:D:82:MET:CE	1:D:114:VAL:HA	2.04	0.86
1:B:22:ASN:O	1:B:26:GLN:HG3	1.76	0.84
1:D:259:ASP:O	1:D:262:LYS:HE3	1.85	0.77
1:B:23:GLN:O	1:B:27:LEU:HD13	1.86	0.76
2:A:401:NAP:H51N	2:A:401:NAP:H2N	1.68	0.75
1:C:44:GLY:HA3	1:C:104:ASP:HB3	1.70	0.72
1:C:72:LEU:HB3	1:C:76:THR:HG21	1.72	0.71
1:D:282:MET:HA	1:D:282:MET:HE2	1.73	0.69
1:D:82:MET:HE1	1:D:114:VAL:HA	1.74	0.68
1:C:73:PRO:O	1:C:76:THR:HG23	1.95	0.67
1:A:19:ARG:HD3	1:A:23:GLN:NE2	2.13	0.64
1:B:6:ILE:HG23	1:B:270:PRO:HD3	1.79	0.63
1:C:37:ARG:NH1	1:C:93:THR:HB	2.14	0.63
1:A:72:LEU:HB3	1:A:76:THR:HG21	1.81	0.62
1:D:201:HIS:HB3	1:D:204:GLU:HG3	1.81	0.61
1:C:24:VAL:HG12	1:C:28:LYS:HE3	1.82	0.61
1:B:110:ASN:HB3	1:B:113:GLU:HB2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ALA:HB1	2:B:401:NAP:H4D	1.84	0.59
1:C:130:ILE:HG13	1:D:130:ILE:HG13	1.84	0.59
1:A:12:ILE:HD13	1:A:158:GLU:HG3	1.86	0.58
1:C:16:ILE:HG23	1:C:19:ARG:HH12	1.69	0.58
1:B:121:GLU:H	1:B:121:GLU:CD	2.11	0.57
1:B:224:GLY:HA3	1:B:260:GLU:HG3	1.85	0.57
1:D:220:GLU:HG2	1:D:257:ALA:HA	1.87	0.56
1:A:35:THR:HG21	1:A:66:LYS:HD2	1.87	0.55
1:C:247:PRO:O	1:C:248:ASN:HB3	2.06	0.55
1:A:44:GLY:HA3	1:A:104:ASP:HB3	1.89	0.54
1:D:225:GLU:CD	1:D:225:GLU:H	2.15	0.54
1:C:20:LEU:O	1:C:24:VAL:HG23	2.07	0.54
1:C:215:ALA:HB1	2:C:401:NAP:H4D	1.91	0.53
1:C:246:LYS:HE2	1:C:251:LYS:HB3	1.89	0.53
1:C:212:LEU:HD23	1:C:233:VAL:HG13	1.91	0.53
1:D:240:TYR:CE1	1:D:252:VAL:HG22	2.44	0.52
1:B:289:GLU:O	1:B:293:ARG:HG3	2.10	0.52
1:C:216:THR:HG21	1:C:221:MET:HE1	1.92	0.52
1:A:16:ILE:HD13	1:A:282:MET:HE1	1.92	0.52
1:B:73:PRO:CG	1:B:76:THR:HG23	2.32	0.51
1:D:82:MET:HE3	1:D:114:VAL:HA	1.90	0.51
1:D:59:ALA:HB3	1:D:284:MET:HE3	1.93	0.51
1:B:78:GLU:HG3	1:B:109:ILE:HG23	1.92	0.51
1:B:144:PHE:HZ	1:B:290:SER:HB3	1.75	0.51
1:A:97:PHE:CZ	1:A:118:ILE:HG23	2.46	0.50
1:A:144:PHE:CZ	1:A:290:SER:HB3	2.46	0.50
1:B:4:ALA:HB2	1:B:265:ALA:O	2.10	0.50
1:D:224:GLY:HA2	1:D:227:ILE:HD12	1.94	0.50
1:D:12:ILE:HD13	1:D:158:GLU:HG3	1.94	0.50
1:D:292:LYS:O	1:D:296:GLU:HG2	2.12	0.50
1:A:121:GLU:H	1:A:121:GLU:CD	2.18	0.50
1:C:243:ASP:OD2	1:C:246:LYS:HD2	2.12	0.49
1:B:144:PHE:CZ	1:B:290:SER:HB3	2.47	0.49
1:D:241:VAL:HB	1:D:242:PRO:HD2	1.94	0.49
1:A:283:LEU:HD23	1:A:284:MET:HE2	1.95	0.49
1:D:181:MET:HE2	1:D:185:LEU:HD21	1.94	0.49
1:C:207:ASN:O	1:C:228:LYS:HB2	2.13	0.48
1:A:17:ARG:HG2	1:A:63:ILE:HD11	1.95	0.48
1:A:125:ASP:HB3	1:A:127:LEU:HG	1.96	0.48
1:A:96:GLY:HA2	1:A:122:LYS:HB3	1.95	0.47
1:A:23:GLN:OE1	1:A:292:LYS:HE3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:VAL:O	1:C:122:LYS:NZ	2.45	0.47
1:A:125:ASP:OD2	3:A:402:A1L22:N33	2.47	0.47
1:B:145:ILE:HG22	1:B:150:LYS:HG3	1.97	0.46
1:C:23:GLN:O	1:C:27:LEU:HD13	2.14	0.46
1:C:250:ARG:HE	1:C:250:ARG:HB3	1.51	0.46
1:B:52:TYR:CE2	2:B:401:NAP:H4N	2.51	0.46
1:D:35:THR:HG21	1:D:66:LYS:HG3	1.98	0.46
1:A:85:ILE:HD11	1:A:114:VAL:HG13	1.98	0.46
1:C:34:PHE:CE1	1:C:295:LEU:HD21	2.51	0.46
1:D:223:LYS:HB2	1:D:226:TRP:NE1	2.31	0.46
1:B:155:LEU:HD21	1:B:278:MET:HG3	1.97	0.45
1:C:125:ASP:O	1:C:127:LEU:HD13	2.15	0.45
1:A:19:ARG:HD3	1:A:23:GLN:HE22	1.82	0.45
1:D:212:LEU:HD23	1:D:233:VAL:HG13	1.99	0.45
1:B:74:ARG:HG2	1:B:104:ASP:O	2.17	0.45
1:C:23:GLN:CG	1:C:292:LYS:HZ1	2.31	0.44
1:B:53:ILE:HG21	1:B:69:HIS:CE1	2.52	0.44
1:B:148:THR:HB	1:B:149:PRO:HD3	1.99	0.44
1:D:221:MET:HB3	1:D:221:MET:HE3	1.85	0.44
1:A:78:GLU:O	1:A:82:MET:HG2	2.17	0.44
1:A:125:ASP:OD2	3:A:402:A1L22:N01	2.50	0.44
1:A:173:ARG:HD2	1:B:187:TRP:CZ3	2.53	0.43
1:C:97:PHE:CZ	1:C:118:ILE:HG23	2.53	0.43
1:A:4:ALA:HB2	1:A:265:ALA:O	2.19	0.43
1:A:208:LYS:NZ	1:B:208:LYS:HD3	2.34	0.42
1:D:175:LYS:HB3	1:D:175:LYS:NZ	2.34	0.42
1:A:73:PRO:HG2	1:A:76:THR:HG23	2.01	0.42
1:B:96:GLY:HA2	1:B:122:LYS:HB3	2.01	0.42
1:A:85:ILE:CD1	1:A:114:VAL:HG13	2.50	0.42
1:B:125:ASP:HB3	1:B:127:LEU:HG	2.01	0.42
1:C:110:ASN:ND2	1:C:113:GLU:HG2	2.35	0.42
1:D:236:CYS:O	2:D:401:NAP:H1D	2.20	0.42
1:D:135:LEU:HD12	1:D:140:LEU:HD11	2.02	0.42
1:C:198:LYS:HA	1:C:198:LYS:HD3	1.88	0.42
1:B:85:ILE:HD11	1:B:114:VAL:HG13	2.01	0.42
1:B:91:ASP:OD1	1:B:93:THR:HG23	2.20	0.42
1:B:293:ARG:HA	1:B:296:GLU:CD	2.45	0.42
1:D:36:PRO:HA	1:D:95:HIS:ND1	2.35	0.42
1:A:221:MET:HE3	1:A:221:MET:HB3	1.90	0.41
1:C:21:LYS:HA	1:C:63:ILE:HG23	2.01	0.41
1:C:110:ASN:O	1:C:114:VAL:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:GLY:HA3	1:D:104:ASP:HB3	2.02	0.41
1:C:247:PRO:C	1:C:249:GLY:H	2.29	0.41
1:D:207:ASN:O	1:D:228:LYS:HB2	2.21	0.41
1:D:240:TYR:CD1	1:D:252:VAL:HG22	2.55	0.41
1:B:71:LYS:HB2	1:B:71:LYS:HE2	1.87	0.41
1:A:98:LEU:HD12	1:A:99:VAL:C	2.45	0.41
1:B:8:ASN:CG	1:B:11:GLU:HB3	2.46	0.41
1:C:246:LYS:CE	1:C:251:LYS:HB3	2.50	0.41
1:B:57:LEU:HD11	1:B:69:HIS:HB2	2.03	0.41
1:B:224:GLY:CA	1:B:260:GLU:HG3	2.50	0.41
1:C:125:ASP:HB3	1:C:127:LEU:HD22	2.02	0.41
1:A:296:GLU:H	1:A:296:GLU:HG2	1.64	0.41
1:A:28:LYS:HG2	1:A:34:PHE:O	2.21	0.40
1:D:52:TYR:O	1:D:56:LYS:HG3	2.22	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	282/308 (92%)	273 (97%)	9 (3%)	0	100	100
1	B	282/308 (92%)	272 (96%)	10 (4%)	0	100	100
1	C	292/308 (95%)	282 (97%)	10 (3%)	0	100	100
1	D	282/308 (92%)	272 (96%)	10 (4%)	0	100	100
All	All	1138/1232 (92%)	1099 (97%)	39 (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	237/260 (91%)	234 (99%)	3 (1%)	61	76
1	B	237/260 (91%)	236 (100%)	1 (0%)	84	91
1	C	244/260 (94%)	238 (98%)	6 (2%)	42	58
1	D	238/260 (92%)	234 (98%)	4 (2%)	53	70
All	All	956/1040 (92%)	942 (98%)	14 (2%)	57	72

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

Mol	Chain	Res	Type
1	A	11	GLU
1	A	108	SER
1	A	115	ILE
1	B	140	LEU
1	C	79	SER
1	C	108	SER
1	C	125	ASP
1	C	127	LEU
1	C	250	ARG
1	C	253	VAL
1	D	23	GLN
1	D	98	LEU
1	D	114	VAL
1	D	125	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	C	54	ASN
1	C	110	ASN
1	C	207	ASN
1	C	248	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	239	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
3	A1L22	A	402	-	34,35,35	2.59	7 (20%)	44,48,48	1.21	4 (9%)
3	A1L22	C	402	-	34,35,35	2.60	9 (26%)	44,48,48	1.41	8 (18%)
2	NAP	C	401	-	50,52,52	1.67	4 (8%)	71,80,80	1.08	7 (9%)
3	A1L22	D	402	-	34,35,35	2.45	11 (32%)	44,48,48	1.39	8 (18%)
2	NAP	B	401	-	50,52,52	1.90	3 (6%)	71,80,80	1.24	4 (5%)
3	A1L22	B	402	-	34,35,35	2.54	10 (29%)	44,48,48	1.34	7 (15%)
2	NAP	D	401	-	50,52,52	1.70	3 (6%)	71,80,80	1.22	7 (9%)
2	NAP	A	401	-	50,52,52	1.81	4 (8%)	71,80,80	1.07	6 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1L22	A	402	-	-	3/25/25/25	0/3/3/3
3	A1L22	C	402	-	-	0/25/25/25	0/3/3/3
2	NAP	C	401	-	-	8/35/67/67	0/5/5/5
3	A1L22	D	402	-	-	4/25/25/25	0/3/3/3
2	NAP	B	401	-	-	7/35/67/67	0/5/5/5
3	A1L22	B	402	-	-	3/25/25/25	0/3/3/3
2	NAP	D	401	-	-	11/35/67/67	0/5/5/5
2	NAP	A	401	-	-	8/35/67/67	0/5/5/5

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	A1L22	O32-C06	9.56	1.41	1.23
3	C	402	A1L22	O32-C06	9.13	1.40	1.23
3	B	402	A1L22	O32-C06	9.04	1.40	1.23
2	A	401	NAP	P2B-O2B	8.45	1.74	1.59
3	D	402	A1L22	O32-C06	8.28	1.39	1.23
2	C	401	NAP	P2B-O2B	8.07	1.73	1.59
2	B	401	NAP	P2B-O2B	7.88	1.73	1.59
2	B	401	NAP	PN-O3	7.30	1.67	1.59
2	D	401	NAP	P2B-O2B	7.19	1.72	1.59
2	B	401	NAP	PA-O3	6.45	1.66	1.59
2	D	401	NAP	PA-O3	5.85	1.65	1.59
2	D	401	NAP	PN-O3	5.66	1.65	1.59
2	A	401	NAP	PN-O3	5.55	1.65	1.59
2	A	401	NAP	PA-O3	5.44	1.65	1.59
3	D	402	A1L22	C02-N33	5.18	1.46	1.34
3	C	402	A1L22	C02-N33	5.16	1.46	1.34
3	C	402	A1L22	C18-N20	5.06	1.45	1.34
3	A	402	A1L22	C04-N11	4.90	1.46	1.34
3	A	402	A1L22	C02-N33	4.73	1.45	1.34
2	C	401	NAP	PN-O3	4.72	1.64	1.59
3	A	402	A1L22	C18-N20	4.68	1.45	1.34
3	B	402	A1L22	C02-N33	4.63	1.45	1.34
3	C	402	A1L22	C04-N11	4.56	1.45	1.34
2	C	401	NAP	PA-O3	4.54	1.64	1.59
3	B	402	A1L22	C18-N20	4.47	1.44	1.34
3	D	402	A1L22	C18-N20	4.32	1.44	1.34
3	D	402	A1L22	C04-N11	4.28	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	A1L22	C04-N11	4.17	1.44	1.34
3	B	402	A1L22	C06-N01	-4.01	1.31	1.38
3	A	402	A1L22	C06-N01	-3.86	1.31	1.38
3	B	402	A1L22	C08-N09	3.81	1.45	1.37
3	C	402	A1L22	C08-N09	3.64	1.45	1.37
3	A	402	A1L22	C08-N09	3.63	1.45	1.37
3	D	402	A1L22	C08-N09	3.56	1.45	1.37
3	C	402	A1L22	C06-N01	-3.50	1.32	1.38
3	D	402	A1L22	C06-N01	-3.21	1.32	1.38
3	C	402	A1L22	C08-N07	2.74	1.45	1.39
3	B	402	A1L22	C26-C27	2.59	1.54	1.49
3	D	402	A1L22	C26-C27	2.43	1.53	1.49
3	A	402	A1L22	O19-C18	-2.39	1.17	1.23
3	B	402	A1L22	C08-N07	2.35	1.44	1.39
3	C	402	A1L22	O12-C08	-2.26	1.18	1.23
3	B	402	A1L22	C02-N01	-2.22	1.32	1.37
3	D	402	A1L22	C08-N07	2.21	1.44	1.39
3	D	402	A1L22	C27-N28	2.08	1.37	1.33
3	D	402	A1L22	C04-N03	-2.07	1.31	1.36
3	B	402	A1L22	C27-N28	2.06	1.37	1.33
2	A	401	NAP	O3B-C3B	-2.06	1.37	1.43
3	D	402	A1L22	C02-N01	-2.04	1.32	1.37
3	C	402	A1L22	C02-N01	-2.03	1.32	1.37
2	C	401	NAP	O4D-C1D	-2.01	1.38	1.40

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAP	O4B-C1B-N9A	4.69	117.10	108.09
2	D	401	NAP	O4B-C1B-N9A	3.48	114.78	108.09
3	A	402	A1L22	C26-C23-C21	-3.46	106.79	113.16
3	B	402	A1L22	C22-C21-N20	-3.39	102.71	110.57
3	D	402	A1L22	O32-C06-C05	-3.34	119.21	127.26
3	D	402	A1L22	C02-N03-C04	3.20	120.42	113.79
2	A	401	NAP	C2B-C1B-N9A	-3.17	108.53	113.75
2	B	401	NAP	O5D-C5D-C4D	3.17	119.78	108.99
3	C	402	A1L22	O32-C06-C05	-3.04	119.93	127.26
3	A	402	A1L22	C23-C21-N20	-2.93	105.11	110.91
2	C	401	NAP	O3X-P2B-O2X	2.82	118.39	107.80
3	B	402	A1L22	O32-C06-C05	-2.82	120.46	127.26
3	B	402	A1L22	C06-C05-N07	-2.82	113.62	118.45
3	C	402	A1L22	C02-N03-C04	2.80	119.58	113.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAP	O4B-C1B-N9A	2.74	113.36	108.09
2	D	401	NAP	P2B-O2B-C2B	-2.74	116.12	123.43
2	D	401	NAP	O3X-P2B-O2X	2.72	118.02	107.80
2	B	401	NAP	O7N-C7N-N7N	2.72	126.55	122.62
3	A	402	A1L22	N11-C04-N03	2.67	121.63	116.23
3	B	402	A1L22	C02-N03-C04	2.53	119.02	113.79
3	C	402	A1L22	N11-C04-N03	2.52	121.33	116.23
3	C	402	A1L22	C26-C23-C21	-2.52	108.52	113.16
2	C	401	NAP	C2B-C1B-N9A	-2.51	109.63	113.75
3	C	402	A1L22	C05-C06-N01	2.49	118.96	112.13
2	D	401	NAP	O2N-PN-O1N	2.44	123.81	112.44
3	C	402	A1L22	C02-N01-C06	-2.43	120.70	125.11
3	D	402	A1L22	C05-C06-N01	2.42	118.77	112.13
2	B	401	NAP	O3X-P2B-O2X	2.41	116.83	107.80
3	B	402	A1L22	C02-N01-C06	-2.40	120.75	125.11
3	B	402	A1L22	O24-C22-C21	2.38	121.57	113.51
3	D	402	A1L22	C02-N01-C06	-2.38	120.80	125.11
3	D	402	A1L22	C22-C21-N20	-2.36	105.09	110.57
2	D	401	NAP	O7N-C7N-N7N	2.30	125.95	122.62
3	D	402	A1L22	C06-C05-N07	2.30	122.39	118.45
2	A	401	NAP	O2D-C2D-C3D	2.28	119.13	111.82
3	D	402	A1L22	O24-C22-C21	2.27	121.19	113.51
2	A	401	NAP	O5D-C5D-C4D	2.27	116.71	108.99
2	D	401	NAP	O2X-P2B-O2B	-2.20	97.26	105.85
2	C	401	NAP	O2X-P2B-O2B	-2.18	97.34	105.85
3	B	402	A1L22	C05-C06-N01	2.18	118.11	112.13
2	C	401	NAP	O2A-PA-O1A	2.15	122.46	112.44
2	D	401	NAP	O3D-C3D-C4D	-2.13	104.96	111.08
3	C	402	A1L22	C23-C21-N20	-2.10	106.76	110.91
2	A	401	NAP	C6N-N1N-C1D	-2.08	115.64	119.73
3	D	402	A1L22	N11-C04-N03	2.07	120.43	116.23
2	C	401	NAP	O2D-C2D-C3D	2.06	118.44	111.82
2	C	401	NAP	O2N-PN-O1N	2.05	121.99	112.44
2	A	401	NAP	O2X-P2B-O2B	-2.04	97.90	105.85
2	A	401	NAP	O2A-PA-O1A	2.03	121.87	112.44
3	C	402	A1L22	N09-C08-N07	2.01	118.58	114.22
3	A	402	A1L22	C02-N03-C04	2.01	117.95	113.79

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	C5D-O5D-PN-O3
2	A	401	NAP	C5D-O5D-PN-O2N
2	B	401	NAP	O4D-C4D-C5D-O5D
2	D	401	NAP	C5D-O5D-PN-O3
2	D	401	NAP	C5D-O5D-PN-O1N
2	D	401	NAP	C5D-O5D-PN-O2N
2	D	401	NAP	O4D-C4D-C5D-O5D
2	D	401	NAP	C3D-C4D-C5D-O5D
2	C	401	NAP	C3B-C4B-C5B-O5B
3	D	402	A1L22	C21-C23-C26-C27
2	C	401	NAP	O4B-C4B-C5B-O5B
3	D	402	A1L22	N20-C21-C23-C26
2	A	401	NAP	C1B-C2B-O2B-P2B
2	B	401	NAP	C1B-C2B-O2B-P2B
2	C	401	NAP	C1B-C2B-O2B-P2B
2	A	401	NAP	C3B-C2B-O2B-P2B
2	B	401	NAP	C3B-C2B-O2B-P2B
2	C	401	NAP	C3B-C2B-O2B-P2B
2	B	401	NAP	C3D-C4D-C5D-O5D
2	A	401	NAP	O4D-C4D-C5D-O5D
3	A	402	A1L22	N20-C21-C23-C26
2	D	401	NAP	C1B-C2B-O2B-P2B
2	A	401	NAP	O4B-C4B-C5B-O5B
2	D	401	NAP	C3B-C2B-O2B-P2B
2	B	401	NAP	O4B-C4B-C5B-O5B
3	D	402	A1L22	C22-C21-C23-C26
3	B	402	A1L22	C23-C26-C27-N28
3	B	402	A1L22	C23-C26-C27-N31
2	D	401	NAP	O4B-C4B-C5B-O5B
2	C	401	NAP	C2B-O2B-P2B-O2X
2	C	401	NAP	O4D-C1D-N1N-C6N
2	A	401	NAP	C2B-O2B-P2B-O1X
2	B	401	NAP	C2B-O2B-P2B-O1X
2	D	401	NAP	C2B-O2B-P2B-O1X
3	A	402	A1L22	C21-C23-C26-C27
3	B	402	A1L22	N20-C21-C23-C26
3	D	402	A1L22	C23-C26-C27-N31
2	A	401	NAP	PN-O3-PA-O1A
2	C	401	NAP	PN-O3-PA-O1A
2	C	401	NAP	PA-O3-PN-O2N
2	B	401	NAP	C2B-O2B-P2B-O2X
2	D	401	NAP	C2B-O2B-P2B-O2X
2	D	401	NAP	C2B-O2B-P2B-O3X

Continued on next page...

Continued from previous page...

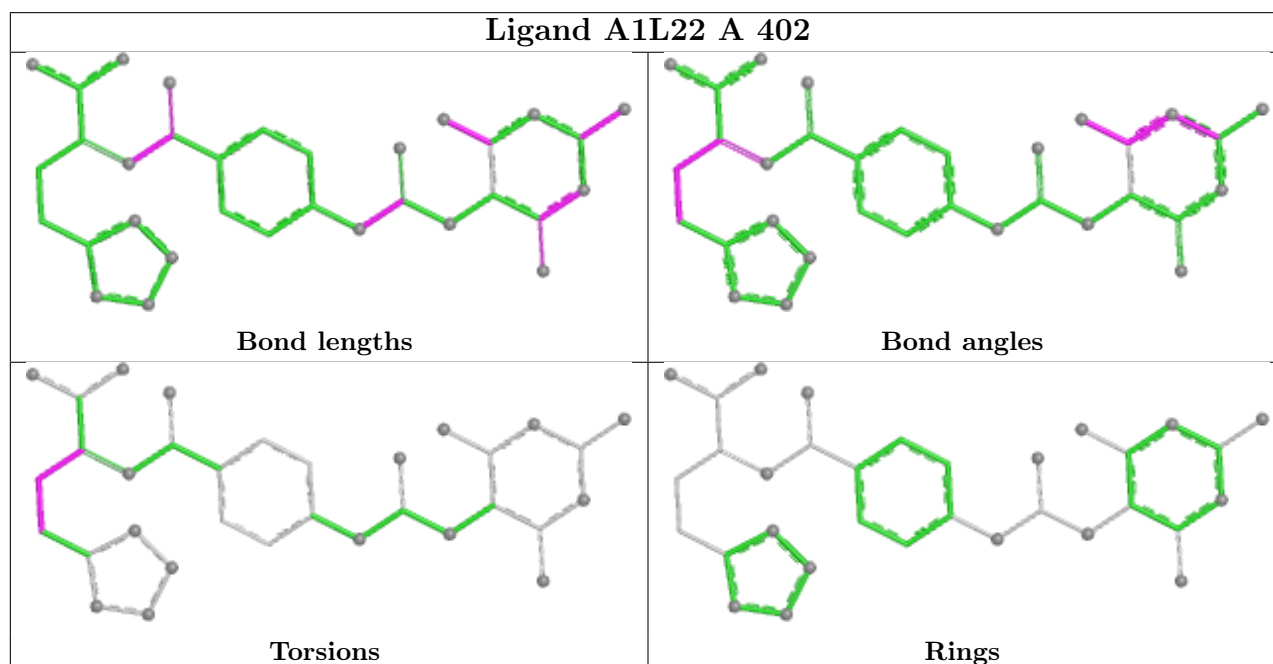
Mol	Chain	Res	Type	Atoms
3	A	402	A1L22	C22-C21-C23-C26

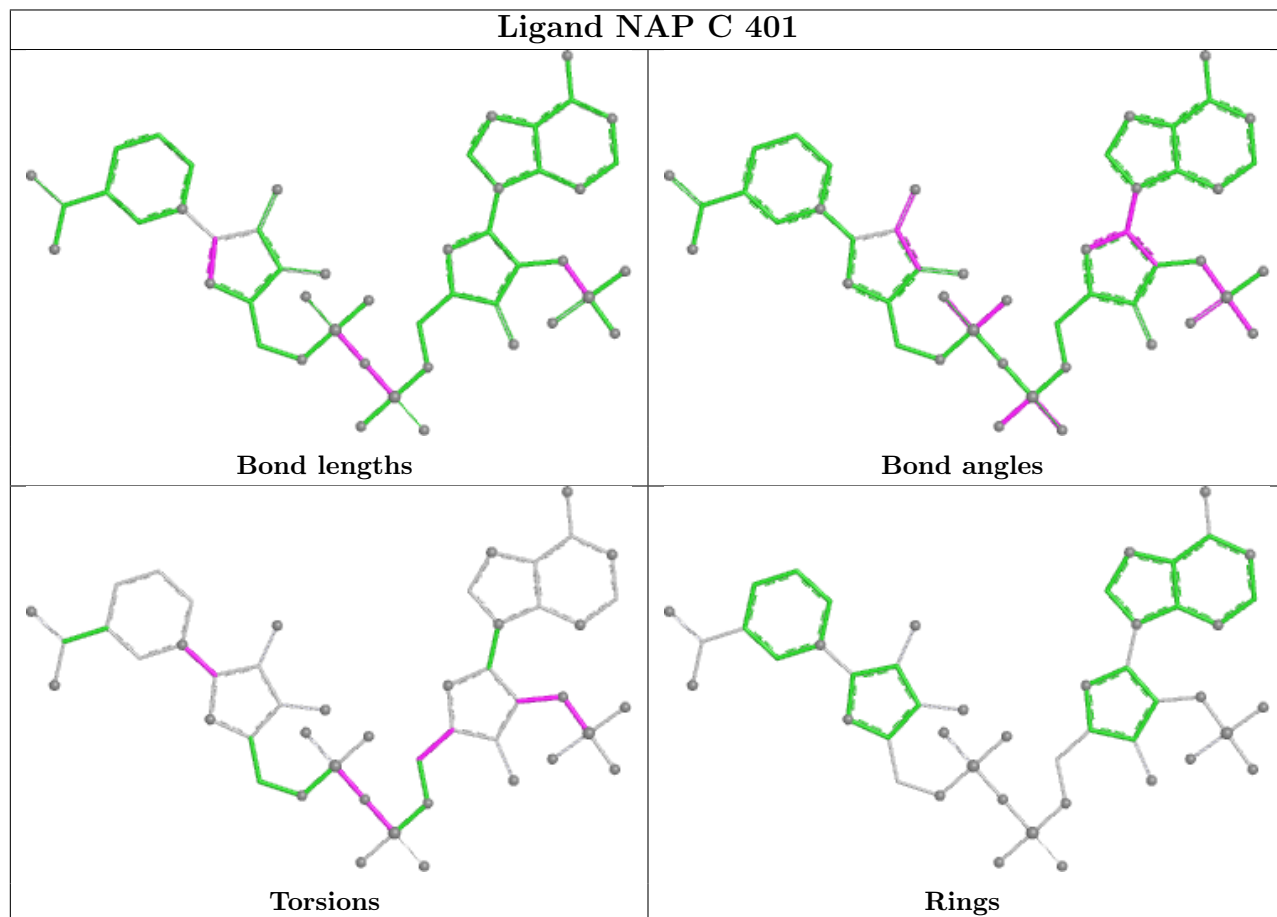
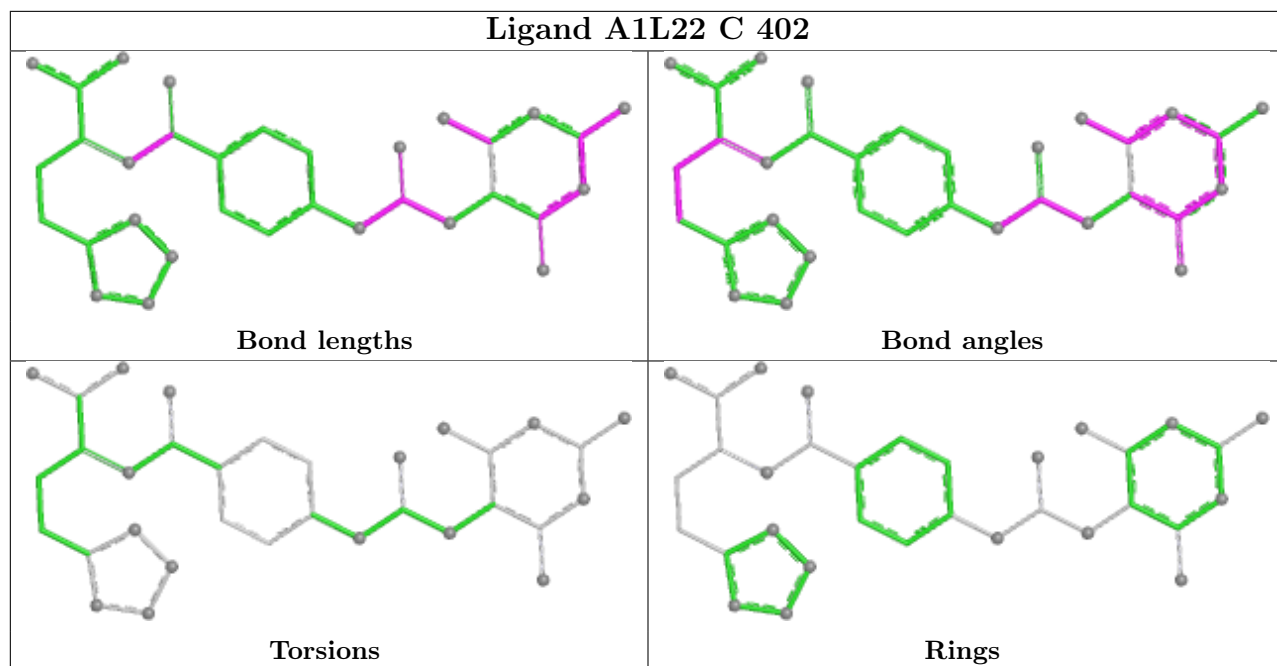
There are no ring outliers.

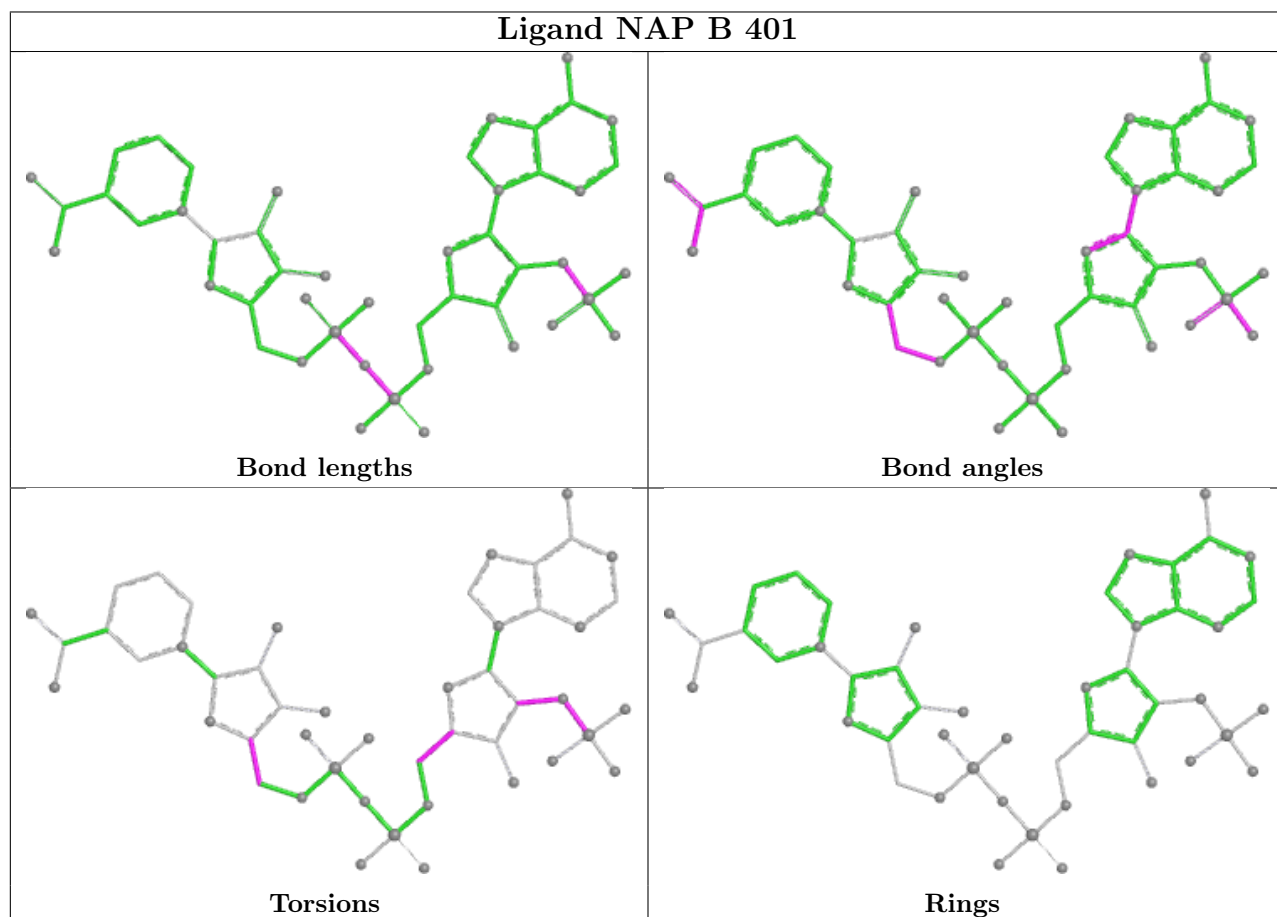
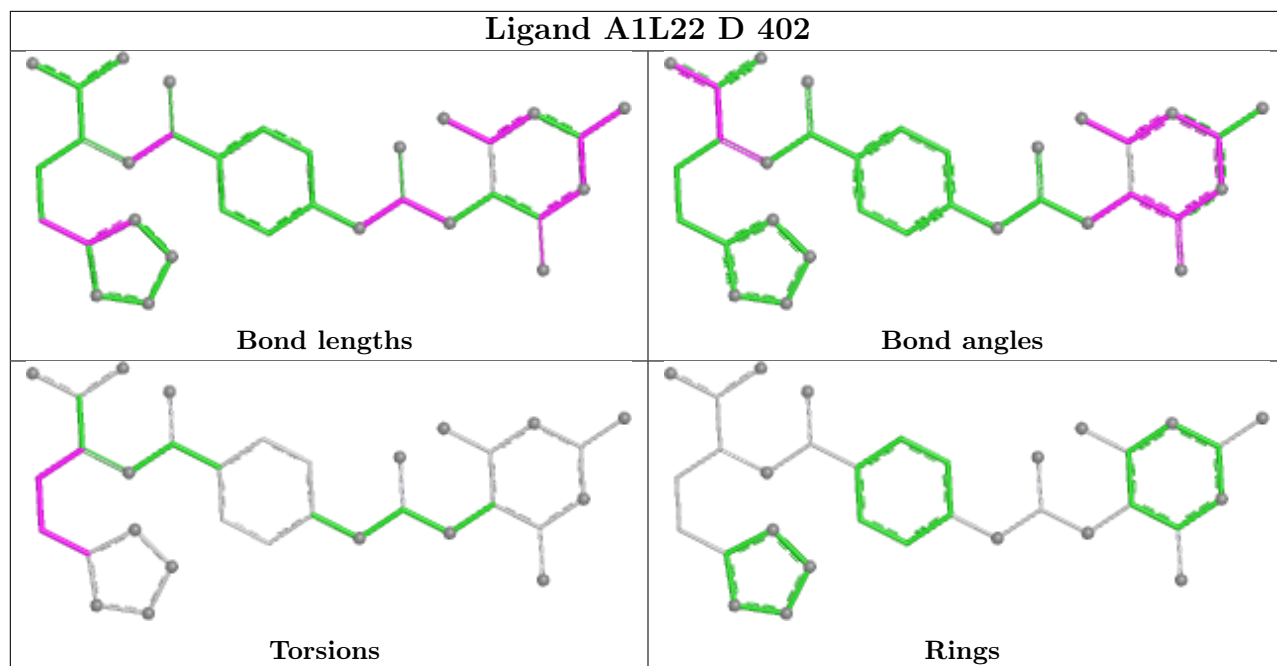
5 monomers are involved in 7 short contacts:

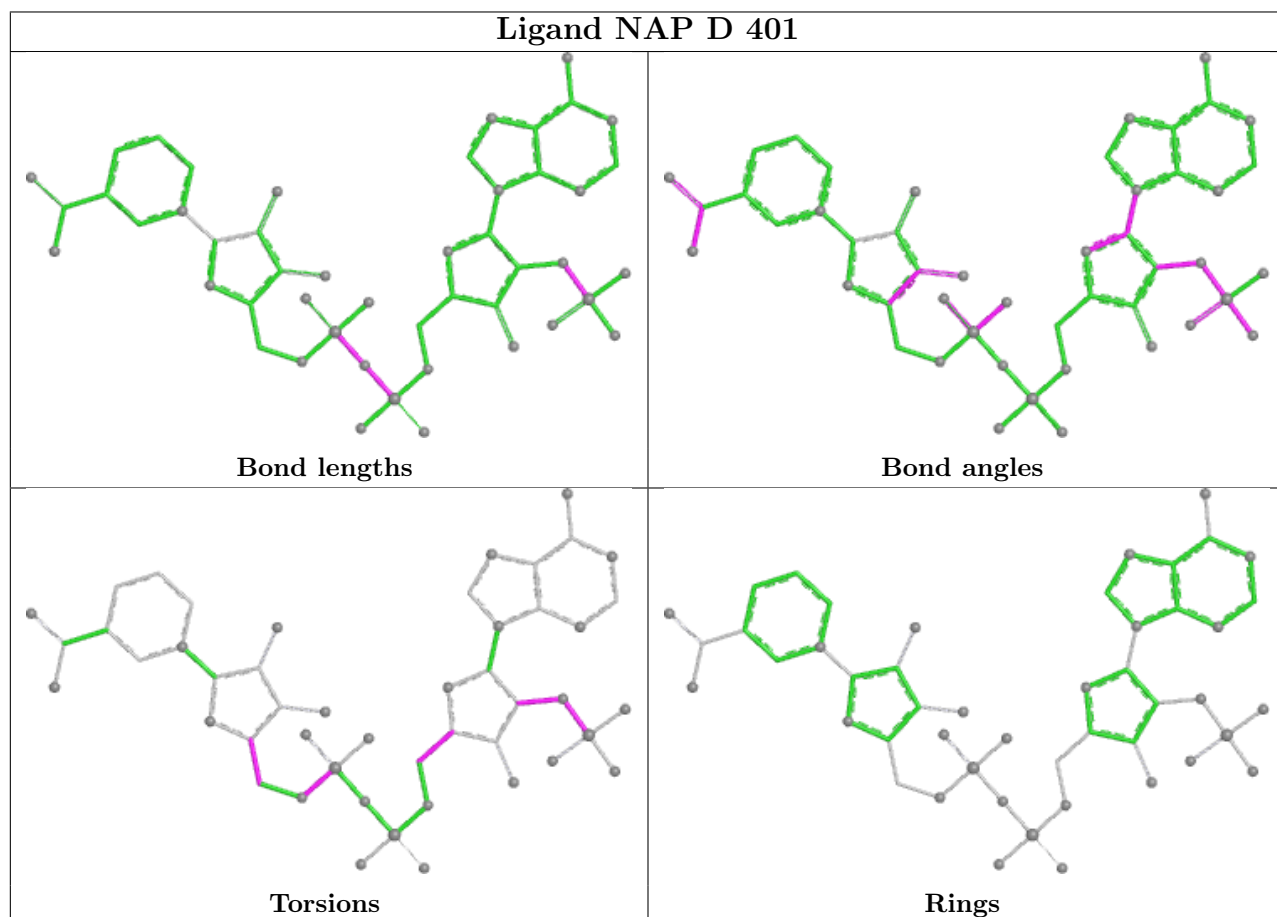
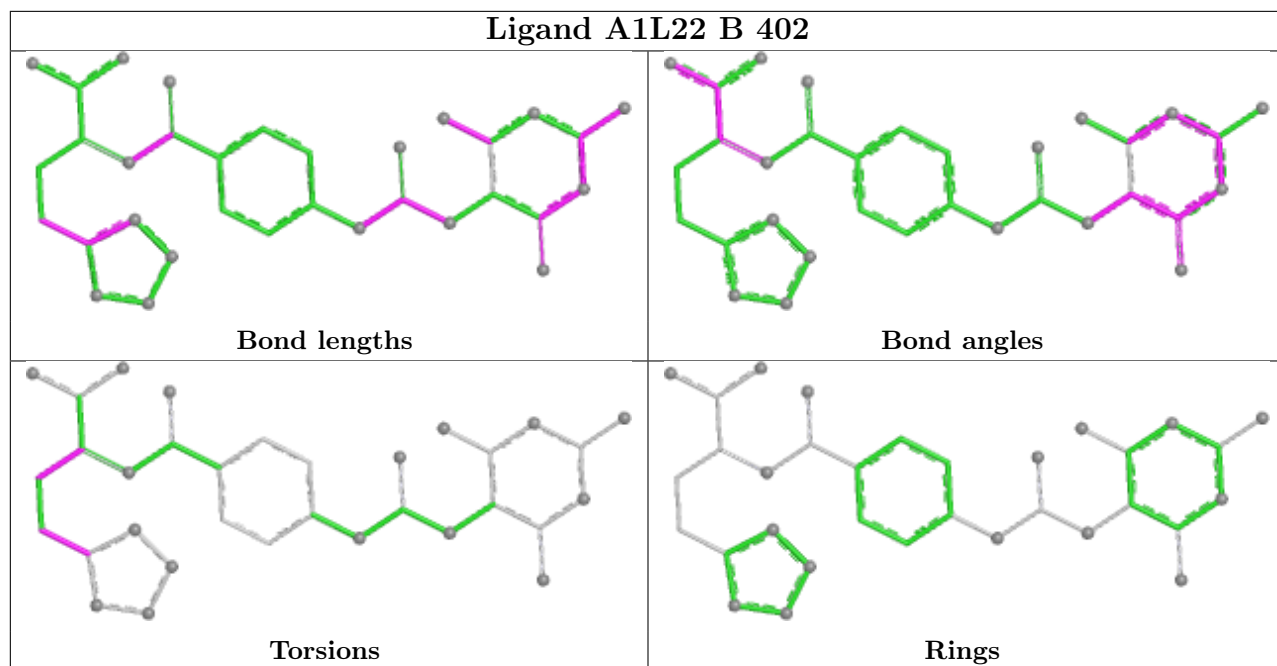
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	A1L22	2	0
2	C	401	NAP	1	0
2	B	401	NAP	2	0
2	D	401	NAP	1	0
2	A	401	NAP	1	0

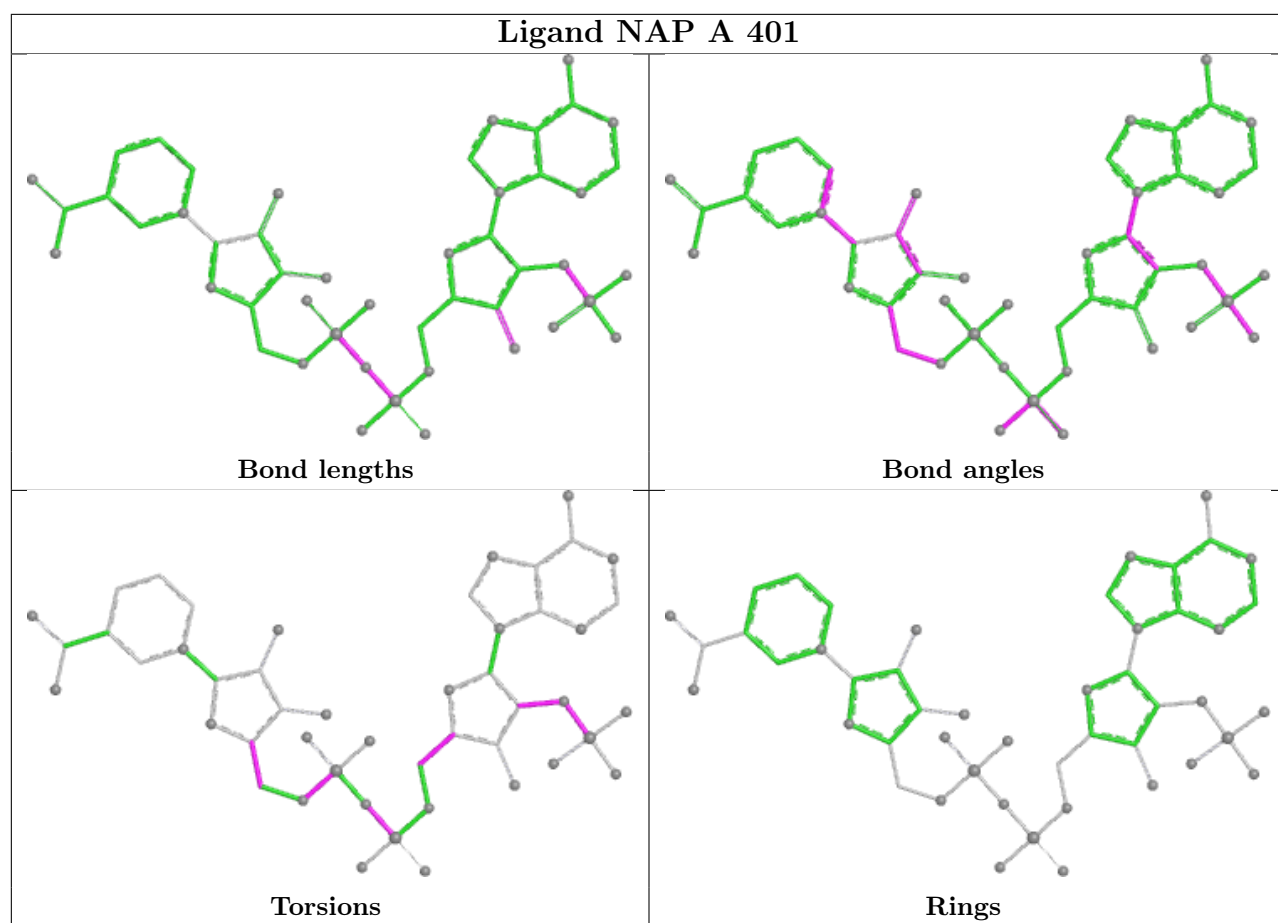
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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	286/308 (92%)	0.13	4 (1%) 73 75	21, 35, 54, 70	0
1	B	286/308 (92%)	0.25	8 (2%) 55 56	23, 38, 61, 75	0
1	C	294/308 (95%)	0.26	3 (1%) 79 81	24, 38, 62, 74	0
1	D	286/308 (92%)	0.49	3 (1%) 79 81	30, 44, 63, 76	0
All	All	1152/1232 (93%)	0.28	18 (1%) 70 72	21, 39, 61, 76	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	GLY	4.8
1	C	244	ASP	3.6
1	C	247	PRO	3.1
1	D	3	PRO	3.1
1	B	296	GLU	3.0
1	B	142	ASP	2.9
1	B	294	PHE	2.8
1	A	141	ASN	2.4
1	D	240	TYR	2.3
1	B	295	LEU	2.3
1	B	26	GLN	2.3
1	A	242	PRO	2.3
1	A	33	GLY	2.2
1	C	248	ASN	2.2
1	A	3	PRO	2.1
1	B	27	LEU	2.1
1	D	271	VAL	2.0
1	B	32	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](#)

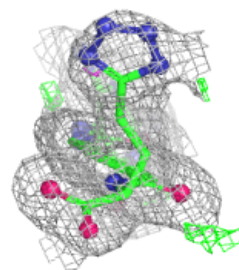
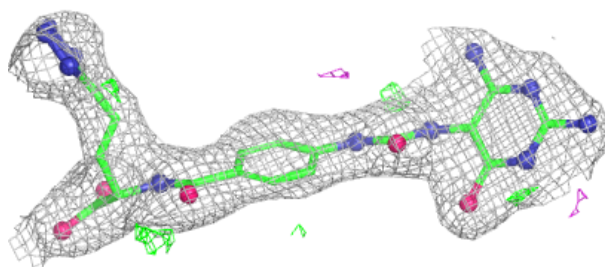
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	A1L22	A	402	33/33	0.92	0.09	27,34,65,68	0
3	A1L22	C	402	33/33	0.92	0.09	31,37,54,55	0
3	A1L22	D	402	33/33	0.92	0.11	30,43,77,78	0
2	NAP	C	401	48/48	0.93	0.10	25,44,55,64	0
3	A1L22	B	402	33/33	0.93	0.09	29,40,55,57	0
2	NAP	D	401	48/48	0.94	0.09	32,50,57,60	0
2	NAP	A	401	48/48	0.95	0.08	27,41,49,52	0
2	NAP	B	401	48/48	0.95	0.08	20,39,55,62	0

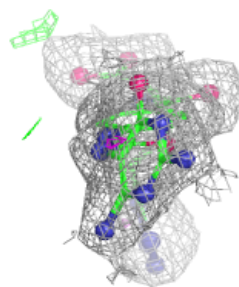
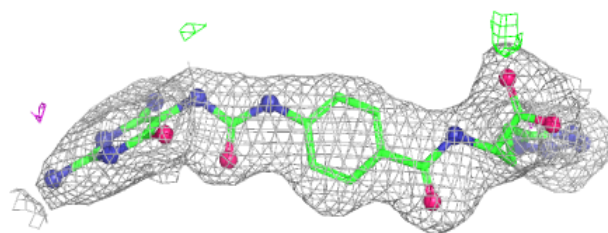
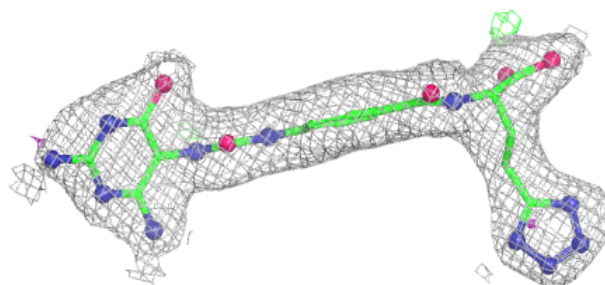
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1L22 A 402:

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

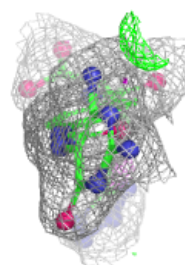
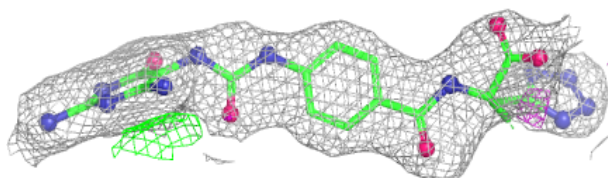
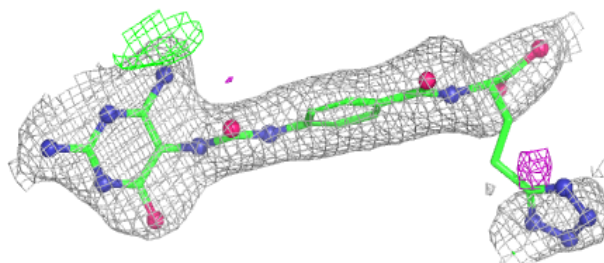
**Electron density around A1L22 C 402:**

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

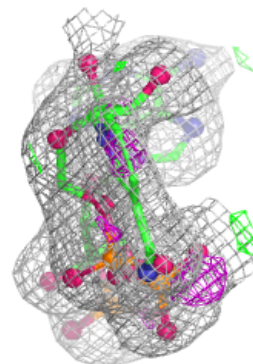
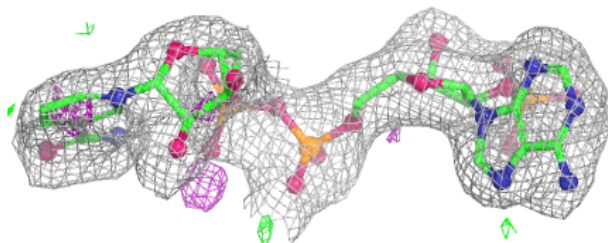
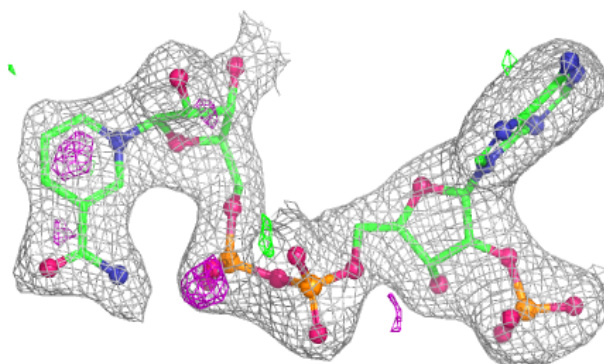


Electron density around A1L22 D 402:

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

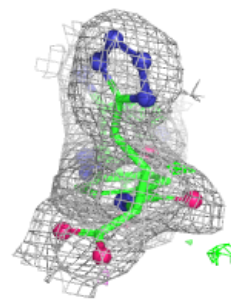
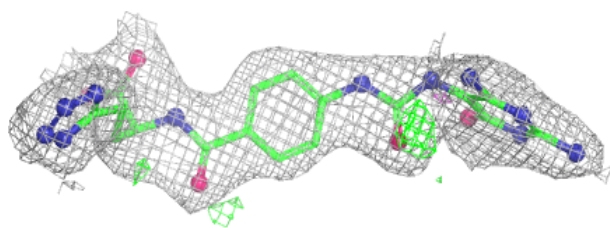
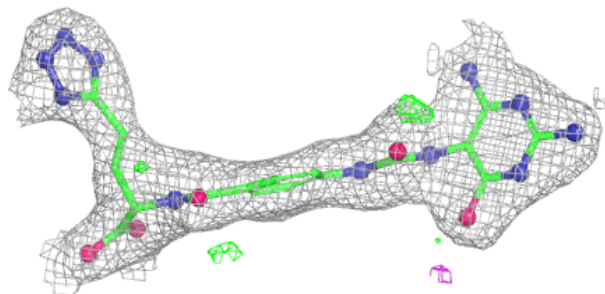
**Electron density around NAP C 401:**

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

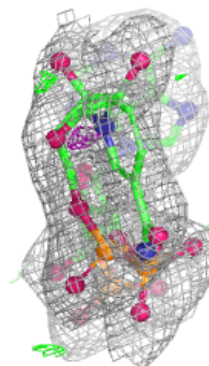
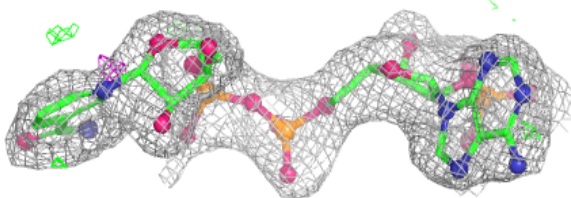
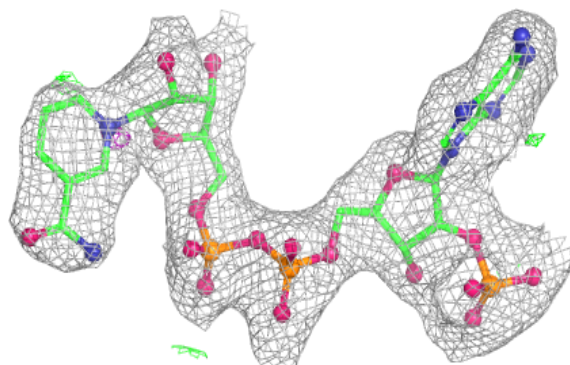


Electron density around A1L22 B 402:

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

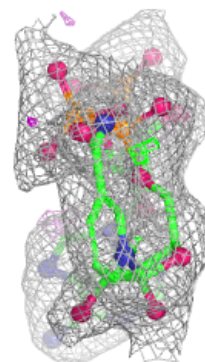
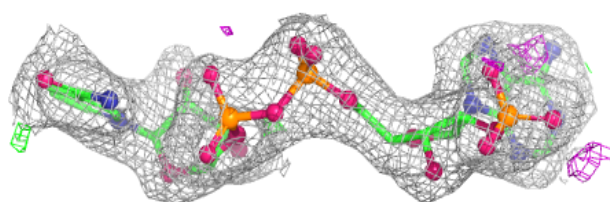
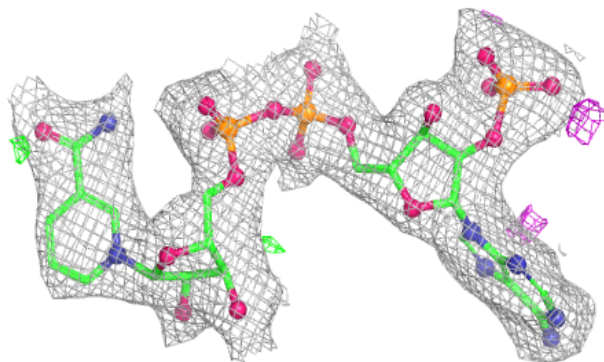
**Electron density around NAP D 401:**

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

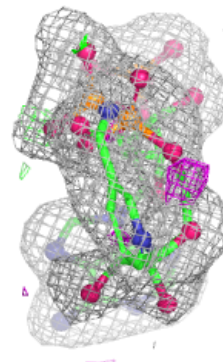
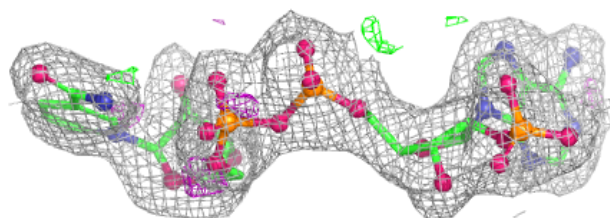
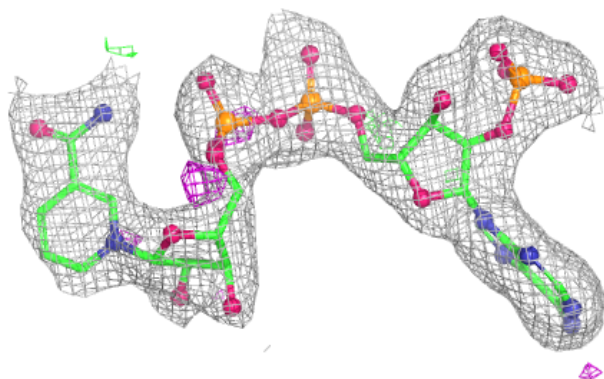


Electron density around NAP A 401:

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

**Electron density around NAP B 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.