



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2021 – 08:38 PM JST

PDB ID : 5B3V
Title : Crystal structure of biliverdin reductase in complex with biliverdin and NADP⁺ from *Synechocystis* sp. PCC 6803
Authors : Takao, H.; Wada, K.
Deposited on : 2016-03-13
Resolution : 2.59 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

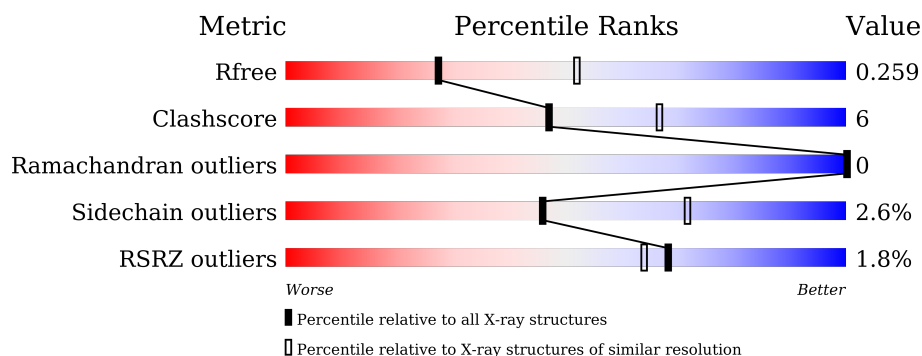
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	331	<div> <div>0%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div> </div>
1	B	331	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	C	331	<div> <div>0%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>5%</div> </div> </div>
1	D	331	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• 5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BLA	B	402	-	-	-	X
3	BLA	C	403	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10756 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.

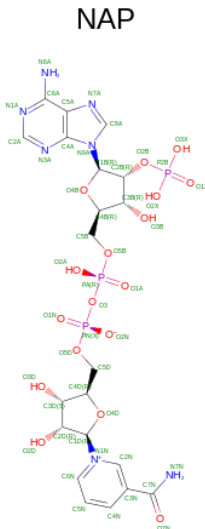
- Molecule 1 is a protein called Biliverdin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	316	Total	C	N	O	S	0	0	0
			2497	1590	446	455	6			
1	A	317	Total	C	N	O	S	0	0	0
			2502	1593	447	456	6			
1	C	316	Total	C	N	O	S	0	0	0
			2497	1590	446	455	6			
1	D	316	Total	C	N	O	S	0	0	0
			2497	1590	446	455	6			

There are 12 discrepancies between the modelled and reference sequences:

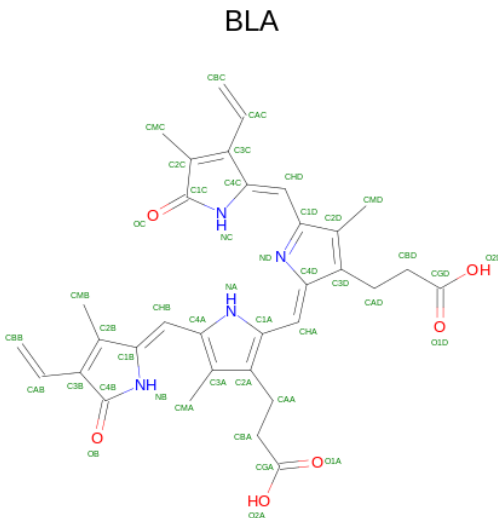
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P72782
B	-1	SER	-	expression tag	UNP P72782
B	0	HIS	-	expression tag	UNP P72782
A	-2	GLY	-	expression tag	UNP P72782
A	-1	SER	-	expression tag	UNP P72782
A	0	HIS	-	expression tag	UNP P72782
C	-2	GLY	-	expression tag	UNP P72782
C	-1	SER	-	expression tag	UNP P72782
C	0	HIS	-	expression tag	UNP P72782
D	-2	GLY	-	expression tag	UNP P72782
D	-1	SER	-	expression tag	UNP P72782
D	0	HIS	-	expression tag	UNP P72782

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 3 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			43	33	4	6		
3	B	1	Total	C	N	O	0	0
			43	33	4	6		
3	A	1	Total	C	N	O	0	0
			43	33	4	6		
3	A	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	0
			43	33	4	6		
3	D	1	Total	C	N	O	0	0
			43	33	4	6		
3	D	1	Total	C	N	O	0	0
			43	33	4	6		

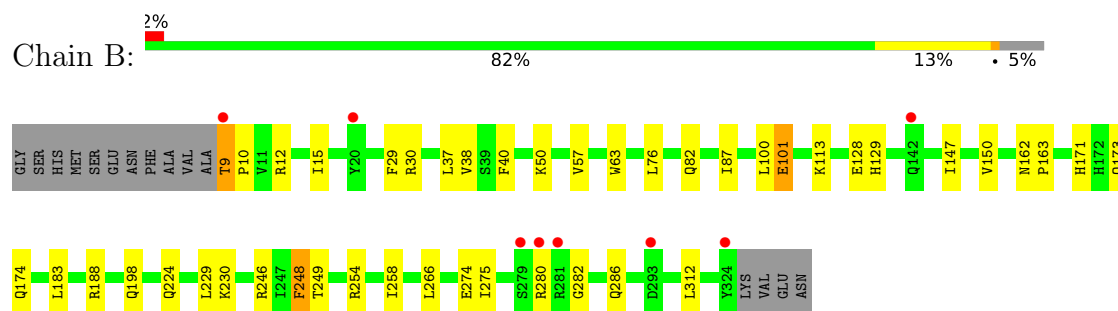
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	56	Total	O	0	0
			56	56		
4	A	71	Total	O	0	0
			71	71		
4	C	45	Total	O	0	0
			45	45		
4	D	55	Total	O	0	0
			55	55		

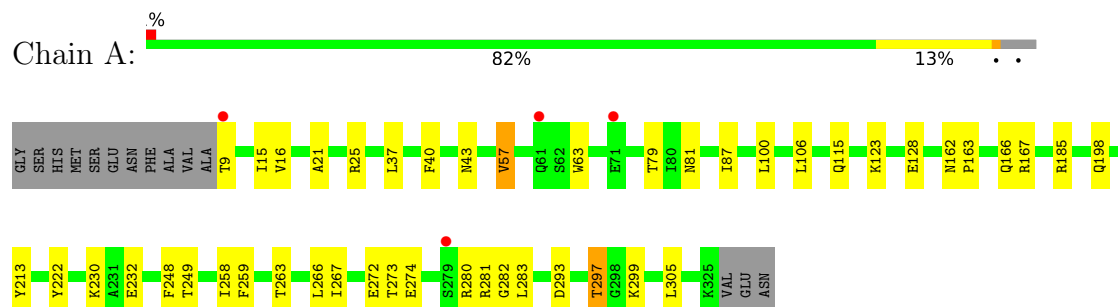
3 Residue-property plots

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.

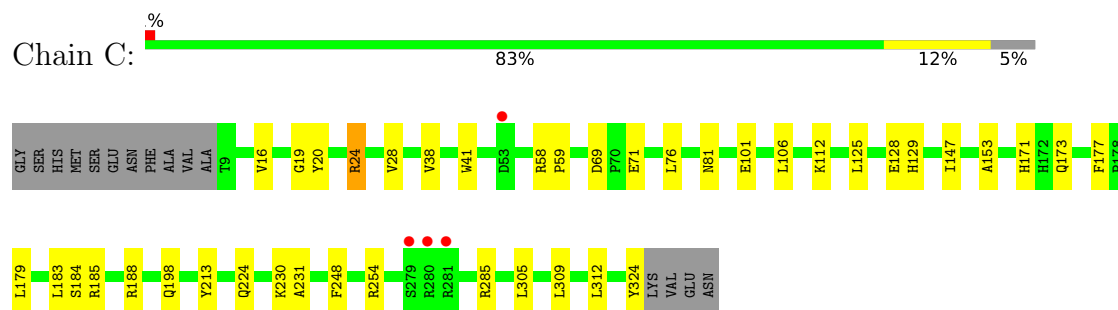
• Molecule 1: Biliverdin reductase



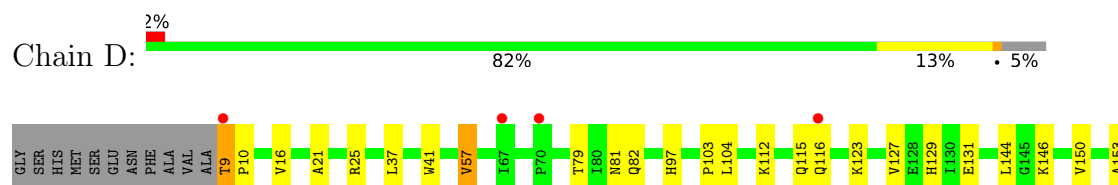
• Molecule 1: Biliverdin reductase



• Molecule 1: Biliverdin reductase



• Molecule 1: Biliverdin reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.50Å 100.41Å 138.03Å 90.00° 95.53° 90.00°	Depositor
Resolution (Å)	49.62 – 2.59 49.63 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.62-2.59) 99.1 (49.63-2.59)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.208 , 0.258 0.208 , 0.259	Depositor DCC
R_{free} test set	2216 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10756	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.02% 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, BLA

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	0.28	0/2557	0.50	0/3467
1	B	0.37	0/2552	0.51	0/3460
1	C	0.37	0/2552	0.55	0/3460
1	D	0.29	0/2552	0.50	0/3460
All	All	0.33	0/10213	0.52	0/13847

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2502	0	2467	24	0
1	B	2497	0	2465	27	0
1	C	2497	0	2465	23	0
1	D	2497	0	2465	24	0
2	A	48	0	24	3	0
2	B	48	0	25	1	0
2	C	48	0	24	3	0
2	D	48	0	25	1	0
3	A	86	0	64	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	86	0	64	11	0
3	C	86	0	64	9	0
3	D	86	0	64	7	0
4	A	71	0	0	0	0
4	B	56	0	0	0	0
4	C	45	0	0	0	0
4	D	55	0	0	0	0
All	All	10756	0	10216	128	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 (128) 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)
3:C:402:BLA:HBD2	3:C:403:BLA:HMA2	1.47	0.94
3:C:402:BLA:HBC1	3:C:402:BLA:HMC1	1.58	0.84
3:B:403:BLA:HBC1	3:B:403:BLA:HMC1	1.59	0.83
3:C:403:BLA:HBC1	3:C:403:BLA:HMC1	1.61	0.83
3:D:402:BLA:HMC1	3:D:402:BLA:HBC1	1.61	0.83
3:B:402:BLA:HBB1	3:B:402:BLA:HMB1	1.60	0.82
3:D:403:BLA:HBB1	3:D:403:BLA:HMB1	1.61	0.82
3:C:402:BLA:HMB1	3:C:402:BLA:HBB1	1.61	0.81
3:A:402:BLA:HMC1	3:A:402:BLA:HBC1	1.63	0.80
3:B:402:BLA:HAD2	3:B:403:BLA:HBD2	1.64	0.79
3:A:403:BLA:HMC1	3:A:403:BLA:HBC1	1.63	0.79
1:B:171:HIS:HE1	1:B:173:GLN:HB2	1.46	0.77
1:B:280:ARG:HD2	3:B:402:BLA:HBC2	1.67	0.75
3:B:402:BLA:HHB	3:B:402:BLA:HBC1	1.67	0.75
1:B:101:GLU:HB3	2:B:401:NAP:H1D	1.72	0.72
1:B:9:THR:HG22	1:B:10:PRO:HA	1.71	0.71
1:D:82:GLN:HB2	1:D:174:GLN:HA	1.72	0.71
1:B:171:HIS:CE1	1:B:173:GLN:HB2	2.24	0.71
1:D:37:LEU:HG	1:D:57:VAL:HG11	1.78	0.65
1:D:267:ILE:HG12	1:D:272:GLU:HG3	1.77	0.65
1:B:9:THR:CG2	1:B:10:PRO:HA	2.27	0.64
1:A:37:LEU:HG	1:A:57:VAL:HG11	1.80	0.62
1:C:185:ARG:NH2	3:C:403:BLA:HBA1	2.16	0.61
2:D:401:NAP:H72N	3:D:402:BLA:HB	1.49	0.61
1:A:115:GLN:HG3	1:A:305:LEU:HD23	1.83	0.60
1:D:129:HIS:HE1	1:D:183:LEU:HD22	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASN:HB3	2:A:401:NAP:O3X	2.03	0.59
1:C:58:ARG:HD3	1:C:59:PRO:HD2	1.85	0.59
3:D:403:BLA:HHB	3:D:403:BLA:HBC1	1.85	0.59
1:C:230:LYS:HD2	1:C:230:LYS:N	2.18	0.58
1:C:38:VAL:HG11	1:C:71:GLU:HG3	1.84	0.58
1:C:101:GLU:HB2	2:C:401:NAP:H1D	1.86	0.58
1:B:198:GLN:HB3	1:B:224:GLN:HB2	1.86	0.57
1:A:81:ASN:HB3	1:A:106:LEU:HD21	1.85	0.57
1:D:150:VAL:HG11	1:D:250:LEU:HD23	1.87	0.57
1:D:266:LEU:HB2	1:D:275:ILE:HD11	1.88	0.55
1:A:79:THR:HA	2:A:401:NAP:H4B	1.89	0.55
1:B:9:THR:HA	1:B:10:PRO:C	2.28	0.53
1:A:9:THR:HG23	1:A:9:THR:O	2.07	0.53
1:C:19:GLY:HA3	2:C:401:NAP:O1A	2.08	0.53
1:B:37:LEU:HG	1:B:57:VAL:HG21	1.90	0.53
1:C:112:LYS:HD3	1:C:309:LEU:HD21	1.89	0.52
1:D:281:ARG:HB3	1:D:282:GLY:HA3	1.90	0.52
1:B:249:THR:HG23	1:B:258:ILE:HG12	1.90	0.52
1:B:12:ARG:HB3	1:B:38:VAL:HG21	1.90	0.52
1:A:281:ARG:HB3	1:A:282:GLY:HA3	1.92	0.52
1:B:129:HIS:HE1	1:B:183:LEU:HD23	1.75	0.52
1:A:222:TYR:HB3	1:A:230:LYS:NZ	2.25	0.52
1:A:222:TYR:HD1	1:A:232:GLU:HG2	1.76	0.51
1:D:16:VAL:HG12	1:D:79:THR:HB	1.92	0.51
1:A:297:THR:HG22	1:A:299:LYS:H	1.76	0.50
1:A:249:THR:HG23	1:A:258:ILE:HG12	1.94	0.49
1:B:29:PHE:HE2	1:B:76:LEU:HD13	1.78	0.49
1:A:293:ASP:O	1:A:297:THR:HB	2.13	0.49
1:A:222:TYR:HB3	1:A:230:LYS:HZ2	1.79	0.48
3:D:402:BLA:C3A	3:D:403:BLA:HMA2	2.44	0.48
1:A:185:ARG:HH22	3:A:403:BLA:HBA1	1.79	0.48
1:C:184:SER:O	1:C:188:ARG:HG3	2.14	0.47
3:C:403:BLA:HB	3:C:403:BLA:HA	1.62	0.47
1:D:112:LYS:HE2	1:D:116:GLN:OE1	2.14	0.47
1:B:150:VAL:HG12	1:B:229:LEU:HD13	1.96	0.47
1:D:97:HIS:CE1	1:D:123:LYS:HE2	2.49	0.47
3:C:402:BLA:CBD	3:C:403:BLA:HMA2	2.34	0.47
1:D:202:GLN:HE22	1:D:222:TYR:HE2	1.58	0.47
2:A:401:NAP:H72N	3:A:402:BLA:HB	1.62	0.47
3:C:403:BLA:HBB1	3:C:403:BLA:OB	2.14	0.47
1:D:146:LYS:HA	1:D:254:ARG:NH2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:HIS:HE1	1:C:183:LEU:HD23	1.79	0.47
3:D:403:BLA:HBC1	3:D:403:BLA:CHD	2.45	0.47
1:A:63:TRP:CD2	1:A:87:ILE:HG12	2.49	0.47
1:D:220:THR:HG22	1:D:234:ILE:HD12	1.96	0.47
1:B:82:GLN:HB2	1:B:174:GLN:HA	1.96	0.46
1:A:16:VAL:HG11	1:A:87:ILE:HD13	1.97	0.46
1:C:28:VAL:HG21	1:C:285:ARG:HA	1.96	0.46
1:C:125:LEU:HD23	1:C:305:LEU:HD21	1.98	0.46
1:C:81:ASN:HB3	1:C:106:LEU:HD21	1.97	0.46
1:A:123:LYS:HE3	1:A:123:LYS:HB3	1.82	0.45
1:A:166:GLN:HG2	1:A:213:TYR:CG	2.52	0.45
1:B:40:PHE:HD2	1:B:57:VAL:HG12	1.81	0.45
1:B:15:ILE:O	1:B:40:PHE:HA	2.16	0.45
2:C:401:NAP:H72N	3:C:402:BLA:HC	1.65	0.45
1:A:267:ILE:HG12	1:A:272:GLU:HG3	1.99	0.45
1:D:21:ALA:O	1:D:25:ARG:HG2	2.17	0.45
1:A:162:ASN:HA	1:A:163:PRO:HA	1.81	0.44
1:D:16:VAL:HG13	1:D:41:TRP:HE3	1.82	0.44
3:B:403:BLA:HBB1	3:B:403:BLA:OB	2.17	0.44
1:C:177:PHE:CE2	1:C:179:LEU:HB2	2.53	0.44
3:A:403:BLA:OB	3:A:403:BLA:HBB1	2.18	0.43
1:C:171:HIS:HD2	1:C:213:TYR:CZ	2.36	0.43
1:D:81:ASN:OD1	1:D:103:PRO:HD2	2.18	0.43
3:B:403:BLA:HMC1	3:B:403:BLA:CB	2.41	0.43
1:C:198:GLN:HB3	1:C:224:GLN:HB2	2.01	0.43
3:B:402:BLA:HBC1	3:B:402:BLA:CHD	2.43	0.43
1:C:171:HIS:CE1	1:C:173:GLN:HB2	2.54	0.43
1:D:131:GLU:HB2	1:D:188:ARG:NH1	2.34	0.43
1:D:104:LEU:HB2	1:D:127:VAL:HG21	2.00	0.43
1:B:101:GLU:HG3	1:B:128:GLU:OE1	2.19	0.42
1:C:69:ASP:OD2	1:C:71:GLU:HG2	2.19	0.42
1:D:16:VAL:HG13	1:D:41:TRP:CE3	2.54	0.42
1:B:188:ARG:HD3	1:B:248:PHE:HE1	1.84	0.42
1:B:63:TRP:CE3	1:B:87:ILE:HG12	2.53	0.42
1:B:282:GLY:O	1:B:286:GLN:HG3	2.19	0.42
1:A:266:LEU:HB3	1:A:273:THR:HB	2.01	0.42
1:C:147:ILE:C	1:C:254:ARG:HB2	2.39	0.42
1:D:153:ALA:O	1:D:231:ALA:HA	2.19	0.42
1:B:183:LEU:HD11	1:B:312:LEU:HA	2.00	0.42
3:B:402:BLA:HHB	3:B:402:BLA:HMA1	1.80	0.42
3:B:402:BLA:HMC1	3:B:402:BLA:HAC	1.81	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ILE:O	1:A:40:PHE:HA	2.20	0.42
1:A:259:PHE:HA	1:A:263:THR:O	2.20	0.42
1:B:147:ILE:C	1:B:254:ARG:HB2	2.40	0.41
1:B:266:LEU:HB2	1:B:275:ILE:HD11	2.02	0.41
1:B:162:ASN:HA	1:B:163:PRO:HA	1.94	0.41
1:C:20:TYR:O	1:C:24:ARG:HG2	2.19	0.41
1:D:9:THR:HA	1:D:10:PRO:HD3	1.92	0.41
1:C:183:LEU:HD11	1:C:312:LEU:HA	2.02	0.41
3:A:402:BLA:HHD	3:A:402:BLA:HAC	1.91	0.41
1:C:153:ALA:O	1:C:231:ALA:HA	2.21	0.41
3:D:402:BLA:HMC3	3:D:403:BLA:CHD	2.51	0.41
1:B:113:LYS:HE2	1:B:113:LYS:HB3	1.86	0.41
1:D:169:THR:HA	1:D:175:PHE:CD1	2.56	0.41
3:A:402:BLA:OB	3:A:402:BLA:HBB1	2.21	0.41
1:C:230:LYS:HD2	1:C:230:LYS:H	1.82	0.40
1:B:246:ARG:HD3	3:B:402:BLA:O1D	2.21	0.40
1:A:21:ALA:O	1:A:25:ARG:HG2	2.21	0.40
1:C:16:VAL:HG13	1:C:41:TRP:HE3	1.87	0.40
1:D:295:LEU:HD23	1:D:295:LEU:HA	1.94	0.40
1:D:115:GLN:HG3	1:D:305:LEU:HD23	2.04	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	315/331 (95%)	307 (98%)	8 (2%)	0	100	100
1	B	314/331 (95%)	302 (96%)	12 (4%)	0	100	100
1	C	314/331 (95%)	307 (98%)	7 (2%)	0	100	100
1	D	314/331 (95%)	304 (97%)	10 (3%)	0	100	100
All	All	1257/1324 (95%)	1220 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	255/267 (96%)	245 (96%)	10 (4%)	32	58
1	B	255/267 (96%)	247 (97%)	8 (3%)	40	66
1	C	255/267 (96%)	250 (98%)	5 (2%)	55	78
1	D	255/267 (96%)	251 (98%)	4 (2%)	62	82
All	All	1020/1068 (96%)	993 (97%)	27 (3%)	46	72

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	9	THR
1	B	30	ARG
1	B	50	LYS
1	B	100	LEU
1	B	101	GLU
1	B	230	LYS
1	B	248	PHE
1	B	274	GLU
1	A	57	VAL
1	A	100	LEU
1	A	128	GLU
1	A	167	ARG
1	A	198	GLN
1	A	248	PHE
1	A	274	GLU
1	A	280	ARG
1	A	283	LEU
1	A	297	THR
1	C	24	ARG
1	C	76	LEU
1	C	128	GLU
1	C	248	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	324	TYR
1	D	9	THR
1	D	57	VAL
1	D	144	LEU
1	D	248	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	43	ASN
1	B	174	GLN
1	A	173	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAP	B	401	-	45,52,52	2.01	9 (20%)	56,80,80	4.78	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BLA	B	403	-	36,46,46	5.93	21 (58%)	47,67,67	2.47	8 (17%)
2	NAP	D	401	-	45,52,52	2.01	8 (17%)	56,80,80	4.75	14 (25%)
3	BLA	C	403	-	36,46,46	5.76	22 (61%)	47,67,67	2.49	13 (27%)
3	BLA	D	403	-	36,46,46	5.78	23 (63%)	47,67,67	2.52	9 (19%)
3	BLA	B	402	-	36,46,46	6.22	23 (63%)	47,67,67	3.09	19 (40%)
2	NAP	C	401	-	45,52,52	2.33	12 (26%)	56,80,80	4.26	14 (25%)
3	BLA	D	402	-	36,46,46	5.73	20 (55%)	47,67,67	2.30	11 (23%)
3	BLA	A	402	-	36,46,46	5.76	20 (55%)	47,67,67	2.15	12 (25%)
3	BLA	A	403	-	36,46,46	5.78	22 (61%)	47,67,67	2.43	9 (19%)
3	BLA	C	402	-	36,46,46	5.80	22 (61%)	47,67,67	2.51	10 (21%)
2	NAP	A	401	-	45,52,52	2.31	11 (24%)	56,80,80	4.36	15 (26%)

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	NAP	B	401	-	-	9/31/67/67	0/5/5/5
3	BLA	B	403	-	-	0/22/74/74	0/4/4/4
2	NAP	D	401	-	-	7/31/67/67	0/5/5/5
3	BLA	C	403	-	-	5/22/74/74	0/4/4/4
3	BLA	D	403	-	-	5/22/74/74	0/4/4/4
3	BLA	B	402	-	-	11/22/74/74	0/4/4/4
2	NAP	C	401	-	-	11/31/67/67	0/5/5/5
3	BLA	D	402	-	-	1/22/74/74	0/4/4/4
3	BLA	A	402	-	-	0/22/74/74	0/4/4/4
3	BLA	A	403	-	-	5/22/74/74	0/4/4/4
3	BLA	C	402	-	-	0/22/74/74	0/4/4/4
2	NAP	A	401	-	-	8/31/67/67	0/5/5/5

All (213) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	BLA	CHA-C4D	27.63	1.58	1.35
3	B	403	BLA	CHA-C4D	24.59	1.55	1.35
3	D	403	BLA	CHA-C4D	23.55	1.54	1.35
3	C	402	BLA	CHA-C4D	23.46	1.54	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	BLA	CHA-C4D	23.46	1.54	1.35
3	C	403	BLA	CHA-C4D	23.36	1.54	1.35
3	A	402	BLA	CHA-C4D	23.33	1.54	1.35
3	D	402	BLA	CHA-C4D	23.07	1.54	1.35
3	A	402	BLA	CHB-C1B	9.77	1.54	1.34
3	B	403	BLA	CHB-C1B	9.60	1.54	1.34
3	D	402	BLA	CHB-C1B	9.57	1.54	1.34
3	C	402	BLA	CHB-C1B	9.56	1.54	1.34
3	D	403	BLA	CHB-C1B	9.52	1.54	1.34
3	A	403	BLA	CHB-C1B	9.36	1.53	1.34
3	C	403	BLA	CHB-C1B	8.81	1.52	1.34
3	B	402	BLA	CHB-C1B	8.51	1.52	1.34
3	A	403	BLA	C3C-C4C	-7.78	1.32	1.45
2	B	401	NAP	C3N-C7N	-7.68	1.39	1.50
3	C	402	BLA	C4D-C3D	-7.60	1.33	1.45
2	A	401	NAP	C3N-C7N	-7.52	1.39	1.50
3	D	403	BLA	C4D-C3D	-7.52	1.33	1.45
3	D	402	BLA	C3C-C4C	-7.46	1.33	1.45
2	D	401	NAP	C3N-C7N	-7.44	1.39	1.50
3	D	402	BLA	C4D-C3D	-7.39	1.34	1.45
2	C	401	NAP	C3N-C7N	-7.35	1.39	1.50
3	A	403	BLA	C4D-C3D	-7.34	1.34	1.45
3	A	402	BLA	C3C-C4C	-7.33	1.33	1.45
3	C	403	BLA	C4D-C3D	-7.27	1.34	1.45
3	C	403	BLA	C3C-C4C	-7.21	1.33	1.45
3	A	402	BLA	C4D-C3D	-7.19	1.34	1.45
3	B	403	BLA	C3C-C4C	-7.11	1.33	1.45
3	B	403	BLA	C4D-C3D	-7.09	1.34	1.45
3	C	402	BLA	C3C-C4C	-7.01	1.33	1.45
3	A	403	BLA	OB-C4B	6.92	1.36	1.23
3	C	403	BLA	OB-C4B	6.89	1.36	1.23
3	D	403	BLA	CHD-C4C	6.87	1.54	1.38
3	A	403	BLA	OC-C1C	6.86	1.36	1.23
3	D	402	BLA	OB-C4B	6.85	1.36	1.23
3	D	403	BLA	OB-C4B	6.85	1.36	1.23
3	C	403	BLA	C1B-C2B	-6.85	1.32	1.45
3	B	402	BLA	C1B-C2B	-6.83	1.32	1.45
3	B	403	BLA	OB-C4B	6.83	1.36	1.23
3	A	402	BLA	OB-C4B	6.82	1.36	1.23
3	C	403	BLA	OC-C1C	6.82	1.36	1.23
3	B	402	BLA	CHD-C4C	6.82	1.54	1.38
3	A	402	BLA	OC-C1C	6.80	1.36	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	BLA	OB-C4B	6.80	1.36	1.23
3	B	403	BLA	OC-C1C	6.76	1.36	1.23
3	C	402	BLA	CHD-C4C	6.76	1.54	1.38
3	B	402	BLA	OB-C4B	6.75	1.36	1.23
3	B	402	BLA	OC-C1C	6.75	1.36	1.23
3	B	403	BLA	CHD-C4C	6.74	1.54	1.38
3	D	403	BLA	OC-C1C	6.73	1.36	1.23
3	D	402	BLA	OC-C1C	6.72	1.36	1.23
3	C	403	BLA	CHD-C4C	6.72	1.54	1.38
3	A	403	BLA	C1B-C2B	-6.70	1.33	1.45
3	C	402	BLA	OC-C1C	6.66	1.36	1.23
3	B	403	BLA	C1B-C2B	-6.61	1.33	1.45
3	B	402	BLA	C1D-C2D	-6.54	1.31	1.45
3	D	402	BLA	C1B-C2B	-6.53	1.33	1.45
3	A	403	BLA	CHD-C4C	6.52	1.53	1.38
3	C	402	BLA	C1B-C2B	-6.49	1.33	1.45
3	D	403	BLA	C1B-C2B	-6.42	1.33	1.45
3	A	402	BLA	C1B-C2B	-6.40	1.33	1.45
3	D	402	BLA	CHD-C4C	6.39	1.53	1.38
3	A	402	BLA	CHD-C4C	6.29	1.53	1.38
3	B	402	BLA	CHD-C1D	6.23	1.55	1.40
3	A	402	BLA	C1D-C2D	-6.16	1.32	1.45
3	D	403	BLA	C3C-C4C	-6.14	1.35	1.45
3	B	403	BLA	C1D-C2D	-6.12	1.32	1.45
3	A	403	BLA	C1D-C2D	-6.11	1.32	1.45
3	C	402	BLA	CHD-C1D	6.10	1.54	1.40
3	B	403	BLA	CHD-C1D	6.08	1.54	1.40
2	C	401	NAP	C3B-C2B	6.08	1.66	1.52
3	D	402	BLA	C1D-C2D	-6.07	1.32	1.45
3	D	403	BLA	C1D-C2D	-6.06	1.32	1.45
2	A	401	NAP	C3B-C2B	6.06	1.66	1.52
3	C	403	BLA	CHD-C1D	6.03	1.54	1.40
3	B	402	BLA	C4D-C3D	-6.02	1.36	1.45
3	C	403	BLA	C1D-C2D	-5.96	1.33	1.45
3	C	402	BLA	C1D-C2D	-5.95	1.33	1.45
3	D	403	BLA	CHD-C1D	5.83	1.54	1.40
3	B	402	BLA	C3C-C4C	-5.82	1.35	1.45
2	A	401	NAP	C2A-N3A	5.76	1.41	1.32
3	A	402	BLA	CHD-C1D	5.70	1.53	1.40
2	C	401	NAP	O4B-C1B	5.56	1.48	1.41
2	D	401	NAP	C2A-N3A	5.55	1.41	1.32
2	C	401	NAP	C2A-N3A	5.53	1.41	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	BLA	CHD-C1D	5.50	1.53	1.40
3	D	403	BLA	C1C-C2C	-5.44	1.32	1.47
3	A	403	BLA	CHD-C1D	5.41	1.53	1.40
2	B	401	NAP	C2A-N3A	5.41	1.40	1.32
3	B	402	BLA	C1C-C2C	-5.35	1.33	1.47
3	D	402	BLA	C1C-C2C	-5.28	1.33	1.47
3	C	402	BLA	C1C-C2C	-5.27	1.33	1.47
3	A	402	BLA	C1C-C2C	-5.23	1.33	1.47
3	B	403	BLA	C1C-C2C	-5.20	1.33	1.47
3	C	403	BLA	C1C-C2C	-5.15	1.33	1.47
3	A	403	BLA	C1C-C2C	-5.02	1.34	1.47
3	A	403	BLA	CAB-C3B	-4.90	1.34	1.47
3	C	403	BLA	CAB-C3B	-4.90	1.34	1.47
3	D	403	BLA	CBB-CAB	4.83	1.54	1.30
3	B	403	BLA	CAB-C3B	-4.83	1.34	1.47
3	C	402	BLA	CBC-CAC	4.83	1.54	1.30
3	A	402	BLA	CBB-CAB	4.83	1.54	1.30
3	B	402	BLA	CBB-CAB	4.79	1.54	1.30
3	C	402	BLA	C3B-C4B	-4.78	1.33	1.47
3	A	402	BLA	CBC-CAC	4.78	1.54	1.30
3	C	402	BLA	CBB-CAB	4.77	1.53	1.30
3	C	403	BLA	CBC-CAC	4.75	1.53	1.30
3	D	402	BLA	CBC-CAC	4.75	1.53	1.30
3	D	402	BLA	CBB-CAB	4.75	1.53	1.30
3	B	403	BLA	CBC-CAC	4.73	1.53	1.30
3	D	402	BLA	CAB-C3B	-4.71	1.34	1.47
3	B	403	BLA	CBB-CAB	4.71	1.53	1.30
3	A	403	BLA	CAC-C3C	-4.71	1.34	1.47
3	B	402	BLA	CBC-CAC	4.70	1.53	1.30
3	D	403	BLA	C3B-C4B	-4.70	1.33	1.47
3	D	403	BLA	CAC-C3C	-4.69	1.34	1.47
3	C	403	BLA	CBB-CAB	4.69	1.53	1.30
3	B	402	BLA	C3B-C4B	-4.68	1.33	1.47
2	C	401	NAP	C2N-N1N	4.68	1.40	1.35
3	A	402	BLA	CAB-C3B	-4.67	1.34	1.47
3	A	403	BLA	CBB-CAB	4.67	1.53	1.30
3	D	403	BLA	CBC-CAC	4.66	1.53	1.30
3	B	403	BLA	C3B-C4B	-4.59	1.34	1.47
3	B	402	BLA	CAB-C3B	-4.58	1.35	1.47
3	B	403	BLA	CAC-C3C	-4.57	1.35	1.47
3	C	402	BLA	CAB-C3B	-4.52	1.35	1.47
3	A	403	BLA	C3B-C4B	-4.51	1.34	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	BLA	CAC-C3C	-4.51	1.35	1.47
3	B	402	BLA	CAC-C3C	-4.50	1.35	1.47
3	C	402	BLA	CAC-C3C	-4.49	1.35	1.47
3	D	402	BLA	CAC-C3C	-4.49	1.35	1.47
3	A	403	BLA	CBC-CAC	4.49	1.52	1.30
3	D	402	BLA	C3B-C4B	-4.47	1.34	1.47
3	A	402	BLA	C3B-C4B	-4.47	1.34	1.47
3	C	403	BLA	C3B-C4B	-4.46	1.34	1.47
2	A	401	NAP	C2N-N1N	4.45	1.40	1.35
3	D	403	BLA	CAB-C3B	-4.43	1.35	1.47
3	A	402	BLA	CAC-C3C	-4.41	1.35	1.47
2	D	401	NAP	C2N-N1N	4.22	1.40	1.35
2	A	401	NAP	O4B-C1B	4.13	1.46	1.41
2	B	401	NAP	C2N-N1N	4.00	1.39	1.35
3	B	402	BLA	C1A-CHA	3.87	1.56	1.41
3	B	402	BLA	CAA-C2A	3.79	1.57	1.52
3	D	403	BLA	C1A-CHA	3.75	1.55	1.41
3	B	403	BLA	C1A-CHA	3.71	1.55	1.41
3	A	402	BLA	C1A-CHA	3.64	1.55	1.41
3	D	402	BLA	C1A-CHA	3.61	1.55	1.41
3	A	402	BLA	C4A-CHB	3.60	1.55	1.41
3	D	402	BLA	C4A-CHB	3.58	1.55	1.41
3	A	403	BLA	C1A-CHA	3.52	1.54	1.41
3	B	403	BLA	C4A-CHB	3.50	1.54	1.41
2	A	401	NAP	C2A-N1A	3.50	1.40	1.33
3	C	403	BLA	C1A-CHA	3.50	1.54	1.41
3	C	402	BLA	C4A-CHB	3.49	1.54	1.41
2	D	401	NAP	C2A-N1A	3.48	1.40	1.33
3	D	403	BLA	C4A-CHB	3.47	1.54	1.41
3	C	402	BLA	C1A-CHA	3.46	1.54	1.41
2	B	401	NAP	C2A-N1A	3.42	1.40	1.33
2	C	401	NAP	C2A-N1A	3.41	1.40	1.33
3	A	403	BLA	C4A-CHB	3.34	1.54	1.41
3	C	403	BLA	C4A-CHB	3.32	1.54	1.41
3	B	402	BLA	C4A-CHB	3.11	1.53	1.41
2	B	401	NAP	C2D-C1D	-2.80	1.49	1.53
3	B	402	BLA	C1B-NB	-2.70	1.33	1.37
2	A	401	NAP	C6A-C5A	-2.69	1.33	1.43
3	C	402	BLA	C1B-NB	-2.68	1.33	1.37
3	B	403	BLA	C4C-NC	-2.67	1.33	1.37
2	B	401	NAP	C5A-C4A	-2.65	1.33	1.40
3	D	403	BLA	C1B-NB	-2.63	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAP	C6A-C5A	-2.60	1.33	1.43
3	C	402	BLA	C4C-NC	-2.60	1.33	1.37
3	C	403	BLA	C1B-NB	-2.59	1.33	1.37
3	D	402	BLA	C1B-NB	-2.59	1.33	1.37
3	A	403	BLA	C4C-NC	-2.59	1.33	1.37
3	C	403	BLA	C4C-NC	-2.58	1.33	1.37
2	D	401	NAP	C5A-C4A	-2.58	1.34	1.40
3	A	402	BLA	C1B-NB	-2.57	1.33	1.37
2	C	401	NAP	C6A-C5A	-2.57	1.33	1.43
2	B	401	NAP	C6A-C5A	-2.55	1.33	1.43
3	D	402	BLA	C4C-NC	-2.46	1.33	1.37
2	C	401	NAP	C5A-C4A	-2.46	1.34	1.40
3	A	402	BLA	C4C-NC	-2.43	1.33	1.37
3	D	403	BLA	C4C-NC	-2.43	1.33	1.37
3	A	403	BLA	C1B-NB	-2.43	1.33	1.37
3	B	403	BLA	C1B-NB	-2.43	1.33	1.37
3	B	402	BLA	C4C-NC	-2.39	1.33	1.37
2	A	401	NAP	C5A-C4A	-2.36	1.34	1.40
3	A	403	BLA	C3B-C2B	-2.28	1.32	1.37
3	C	403	BLA	C3B-C2B	-2.28	1.32	1.37
3	C	402	BLA	C1C-NC	-2.26	1.33	1.38
2	D	401	NAP	C3B-C2B	-2.21	1.48	1.52
2	B	401	NAP	O4D-C4D	2.20	1.49	1.45
3	D	403	BLA	C1C-NC	-2.20	1.33	1.38
3	B	403	BLA	C3B-C2B	-2.19	1.32	1.37
2	D	401	NAP	C2D-C1D	-2.18	1.50	1.53
2	A	401	NAP	C6N-N1N	2.18	1.40	1.35
3	D	403	BLA	C4D-ND	-2.18	1.33	1.38
2	C	401	NAP	O4D-C4D	2.16	1.49	1.45
3	B	402	BLA	C3D-C2D	-2.15	1.32	1.36
3	A	403	BLA	C3D-C2D	-2.13	1.32	1.36
3	B	402	BLA	C3C-C2C	-2.13	1.33	1.37
2	A	401	NAP	O4D-C4D	2.12	1.49	1.45
3	C	403	BLA	C3D-C2D	-2.11	1.32	1.36
2	C	401	NAP	O4D-C1D	2.11	1.44	1.41
2	C	401	NAP	C6N-N1N	2.08	1.40	1.35
2	B	401	NAP	C6N-N1N	2.08	1.40	1.35
3	D	403	BLA	C3C-C2C	-2.06	1.33	1.37
2	A	401	NAP	C2D-C3D	-2.06	1.47	1.53
2	C	401	NAP	C2D-C1D	-2.05	1.50	1.53
3	C	402	BLA	C4D-ND	-2.01	1.34	1.38

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAP	O4D-C1D-C2D	-20.85	76.46	106.93
2	B	401	NAP	O4D-C1D-C2D	-20.64	76.76	106.93
2	A	401	NAP	O4D-C1D-C2D	-20.39	77.13	106.93
2	D	401	NAP	O4D-C1D-C2D	-20.24	77.34	106.93
2	B	401	NAP	O4B-C1B-C2B	-18.35	74.76	106.59
2	D	401	NAP	O4B-C1B-C2B	-17.88	75.58	106.59
3	C	402	BLA	C1A-CHA-C4D	-12.78	113.55	128.81
3	C	403	BLA	C1A-CHA-C4D	-12.73	113.60	128.81
3	B	403	BLA	C1A-CHA-C4D	-12.61	113.74	128.81
3	A	403	BLA	C1A-CHA-C4D	-12.55	113.81	128.81
3	D	403	BLA	C1A-CHA-C4D	-12.14	114.30	128.81
2	A	401	NAP	C1B-N9A-C4A	11.88	147.51	126.64
3	D	402	BLA	C1A-CHA-C4D	-11.47	115.11	128.81
3	B	402	BLA	C1A-CHA-C4D	-10.27	116.55	128.81
3	A	402	BLA	C1A-CHA-C4D	-10.06	116.80	128.81
2	B	401	NAP	O4B-C4B-C5B	-9.79	77.17	109.37
2	D	401	NAP	O4B-C4B-C5B	-9.69	77.49	109.37
2	A	401	NAP	O4D-C4D-C5D	-9.40	78.46	109.37
2	B	401	NAP	O4D-C4D-C5D	-9.34	78.63	109.37
2	D	401	NAP	O4D-C4D-C5D	-9.31	78.73	109.37
2	C	401	NAP	O4D-C4D-C5D	-9.29	78.80	109.37
2	C	401	NAP	C3B-C2B-C1B	-9.21	85.57	102.89
2	C	401	NAP	C5B-C4B-C3B	-9.16	80.84	115.18
2	A	401	NAP	C3B-C2B-C1B	-9.10	85.77	102.89
2	C	401	NAP	O4D-C4D-C3D	-8.40	88.48	105.11
2	A	401	NAP	C5B-C4B-C3B	-8.00	85.21	115.18
2	D	401	NAP	O4D-C4D-C3D	-7.97	89.34	105.11
2	C	401	NAP	C1B-N9A-C4A	7.91	140.54	126.64
2	B	401	NAP	O4D-C4D-C3D	-7.89	89.51	105.11
2	A	401	NAP	O4D-C4D-C3D	-7.88	89.51	105.11
2	D	401	NAP	O4B-C4B-C3B	-7.43	90.42	105.11
3	D	403	BLA	C4C-CHD-C1D	-7.08	110.79	128.08
3	B	402	BLA	CBA-CAA-C2A	6.90	125.22	112.49
2	B	401	NAP	O4B-C4B-C3B	-6.88	91.50	105.11
3	B	402	BLA	CAA-CBA-CGA	6.85	124.17	112.67
2	D	401	NAP	N3A-C2A-N1A	-6.60	118.36	128.68
2	B	401	NAP	N3A-C2A-N1A	-6.58	118.40	128.68
2	C	401	NAP	N3A-C2A-N1A	-6.49	118.53	128.68
3	C	402	BLA	C4C-CHD-C1D	-6.33	112.62	128.08
3	B	402	BLA	CAD-C3D-C2D	-6.20	116.32	127.88
2	A	401	NAP	N3A-C2A-N1A	-6.19	119.00	128.68
3	B	402	BLA	CAD-C3D-C4D	6.12	135.84	125.01
2	A	401	NAP	O4B-C4B-C3B	-5.91	93.41	105.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAP	C3D-C2D-C1D	-5.89	92.10	100.98
2	D	401	NAP	C3B-C2B-C1B	-5.80	91.98	102.89
2	C	401	NAP	O4B-C4B-C3B	-5.78	93.68	105.11
2	A	401	NAP	C3D-C2D-C1D	-5.63	92.50	100.98
2	A	401	NAP	C5D-C4D-C3D	5.50	135.80	115.18
2	C	401	NAP	C3D-C2D-C1D	-5.50	92.70	100.98
2	D	401	NAP	C5D-C4D-C3D	5.44	135.56	115.18
2	D	401	NAP	C5B-C4B-C3B	5.39	135.37	115.18
2	B	401	NAP	C5D-C4D-C3D	5.35	135.22	115.18
2	B	401	NAP	C3B-C2B-C1B	-5.33	92.86	102.89
2	C	401	NAP	C5D-C4D-C3D	5.24	134.81	115.18
3	B	403	BLA	C4C-CHD-C1D	-5.19	115.39	128.08
2	B	401	NAP	C5B-C4B-C3B	5.07	134.20	115.18
2	B	401	NAP	C3D-C2D-C1D	-4.94	93.54	100.98
3	A	402	BLA	C4C-CHD-C1D	-4.80	116.36	128.08
3	D	402	BLA	C4C-CHD-C1D	-4.71	116.56	128.08
3	B	402	BLA	CHD-C1D-ND	4.35	134.03	124.93
3	C	403	BLA	C4C-CHD-C1D	-4.26	117.66	128.08
3	B	402	BLA	C1B-NB-C4B	-4.26	105.25	110.67
3	A	403	BLA	C4C-CHD-C1D	-4.00	118.31	128.08
3	D	402	BLA	C4C-NC-C1C	-3.98	105.61	110.67
3	A	402	BLA	C4C-NC-C1C	-3.97	105.62	110.67
3	A	403	BLA	C4C-NC-C1C	-3.92	105.67	110.67
3	B	402	BLA	CMA-C3A-C2A	3.75	132.01	124.94
3	C	403	BLA	C4C-NC-C1C	-3.64	106.03	110.67
3	B	402	BLA	CAC-C3C-C4C	3.52	133.75	123.54
3	B	403	BLA	C4C-NC-C1C	-3.49	106.23	110.67
3	C	402	BLA	C1B-NB-C4B	-3.38	106.36	110.67
3	B	402	BLA	C3B-C4B-NB	3.37	110.00	106.19
3	D	403	BLA	CAC-C3C-C4C	3.35	133.25	123.54
3	D	403	BLA	C1B-NB-C4B	-3.26	106.52	110.67
3	C	402	BLA	C4C-NC-C1C	-3.23	106.56	110.67
3	A	403	BLA	CHD-C4C-C3C	-3.22	119.61	127.91
3	B	403	BLA	CAD-C3D-C2D	-3.18	121.95	127.88
3	B	402	BLA	C4C-CHD-C1D	-3.15	120.38	128.08
3	C	403	BLA	C1B-NB-C4B	-3.15	106.66	110.67
3	C	402	BLA	C3B-C4B-NB	3.09	109.68	106.19
2	A	401	NAP	C5A-C6A-N6A	-3.06	115.70	120.35
3	D	403	BLA	C3B-C4B-NB	3.01	109.59	106.19
2	D	401	NAP	C5A-C6A-N6A	-2.98	115.82	120.35
3	B	403	BLA	CAD-C3D-C4D	2.95	130.22	125.01
2	C	401	NAP	C6N-N1N-C2N	-2.94	119.29	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	BLA	C4C-NC-C1C	-2.91	106.97	110.67
3	B	402	BLA	CHD-C1D-C2D	-2.90	117.45	124.90
3	B	402	BLA	CHB-C1B-C2B	-2.88	121.28	126.97
2	B	401	NAP	C5A-C6A-N6A	-2.87	116.00	120.35
2	C	401	NAP	C5A-C6A-N6A	-2.84	116.03	120.35
2	A	401	NAP	C6N-N1N-C2N	-2.83	119.39	121.97
3	B	403	BLA	C1B-NB-C4B	-2.83	107.06	110.67
3	C	403	BLA	CAD-C3D-C2D	-2.83	122.61	127.88
2	B	401	NAP	C2B-C3B-C4B	-2.78	95.95	101.99
3	C	403	BLA	CAD-C3D-C4D	2.78	129.92	125.01
3	B	402	BLA	C1D-C2D-C3D	2.78	109.69	106.51
3	A	403	BLA	C1B-NB-C4B	-2.76	107.15	110.67
3	B	402	BLA	CAC-C3C-C2C	-2.73	119.61	128.60
2	B	401	NAP	C6N-N1N-C2N	-2.72	119.49	121.97
3	D	402	BLA	C1B-NB-C4B	-2.65	107.30	110.67
3	D	402	BLA	CHD-C4C-C3C	-2.64	121.10	127.91
2	A	401	NAP	O5B-C5B-C4B	2.58	117.87	108.99
3	B	402	BLA	C2B-C1B-NB	2.58	110.77	106.99
3	D	403	BLA	CAC-C3C-C2C	-2.57	120.12	128.60
3	A	403	BLA	CHD-C1D-ND	2.57	130.31	124.93
3	C	403	BLA	CHD-C1D-ND	2.56	130.30	124.93
2	A	401	NAP	C3N-C7N-N7N	-2.52	114.73	117.75
2	B	401	NAP	C3N-C7N-N7N	-2.50	114.75	117.75
3	A	402	BLA	C3C-C4C-NC	2.47	110.66	106.80
3	A	402	BLA	C1B-NB-C4B	-2.45	107.54	110.67
2	A	401	NAP	O2B-C2B-C1B	2.44	118.89	110.10
2	D	401	NAP	C3N-C7N-N7N	-2.44	114.82	117.75
3	D	402	BLA	C3C-C4C-NC	2.44	110.61	106.80
3	A	402	BLA	CHD-C4C-C3C	-2.43	121.64	127.91
3	A	402	BLA	CHD-C1D-ND	2.41	129.97	124.93
3	B	402	BLA	CMB-C2B-C1B	-2.33	121.25	124.17
3	D	403	BLA	CAD-C3D-C2D	-2.30	123.59	127.88
3	C	402	BLA	CMB-C2B-C1B	-2.28	121.32	124.17
3	D	403	BLA	CHD-C4C-NC	-2.27	121.18	126.06
3	B	403	BLA	CHA-C4D-ND	-2.27	125.68	128.83
3	A	403	BLA	C3C-C4C-NC	2.27	110.35	106.80
3	B	402	BLA	CHA-C4D-ND	-2.27	125.68	128.83
3	A	402	BLA	CBA-CAA-C2A	2.26	116.66	112.49
2	D	401	NAP	C6N-N1N-C2N	-2.20	119.97	121.97
3	C	403	BLA	C3C-C4C-NC	2.20	110.23	106.80
3	C	402	BLA	CAD-C3D-C2D	-2.19	123.79	127.88
2	C	401	NAP	C3N-C7N-N7N	-2.18	115.14	117.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	BLA	CAD-C3D-C2D	-2.17	123.83	127.88
3	C	402	BLA	CBA-CAA-C2A	2.16	116.47	112.49
3	C	402	BLA	CHB-C1B-C2B	-2.16	122.71	126.97
3	D	402	BLA	OB-C4B-NB	-2.15	120.09	125.08
3	C	403	BLA	CHD-C4C-C3C	-2.14	122.39	127.91
2	C	401	NAP	O2B-P2B-O1X	-2.13	101.16	109.39
3	D	403	BLA	C4C-NC-C1C	-2.13	107.96	110.67
3	A	402	BLA	CAD-C3D-C2D	-2.13	123.92	127.88
2	B	401	NAP	O2B-P2B-O1X	-2.12	101.22	109.39
3	A	402	BLA	OB-C4B-NB	-2.11	120.17	125.08
2	B	401	NAP	C2N-C3N-C4N	2.11	120.65	118.26
3	A	402	BLA	CAD-C3D-C4D	2.11	128.73	125.01
3	C	403	BLA	CMA-C3A-C2A	2.09	128.89	124.94
3	C	403	BLA	CBB-CAB-C3B	-2.06	117.37	127.62
3	B	403	BLA	C3C-C4C-NC	2.06	110.02	106.80
3	A	403	BLA	CAD-C3D-C4D	2.05	128.64	125.01
3	D	402	BLA	CBA-CAA-C2A	2.05	116.27	112.49
3	C	403	BLA	C1D-C2D-C3D	2.05	108.86	106.51
3	C	402	BLA	C3C-C4C-NC	2.03	109.97	106.80
3	A	402	BLA	C3B-C4B-NB	2.03	108.48	106.19
3	D	402	BLA	CAD-C3D-C2D	-2.03	124.10	127.88
3	D	402	BLA	CHD-C1D-ND	2.02	129.17	124.93
3	C	403	BLA	OB-C4B-NB	-2.02	120.39	125.08
3	D	402	BLA	C3B-C4B-NB	2.02	108.47	106.19

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	NAP	C2B-O2B-P2B-O1X
2	B	401	NAP	C5D-O5D-PN-O2N
2	A	401	NAP	C5D-O5D-PN-O2N
2	C	401	NAP	C5B-O5B-PA-O1A
2	C	401	NAP	C5B-O5B-PA-O2A
2	C	401	NAP	C2B-O2B-P2B-O1X
2	C	401	NAP	C5D-O5D-PN-O1N
2	C	401	NAP	C5D-O5D-PN-O2N
2	D	401	NAP	C5D-O5D-PN-O2N
3	B	402	BLA	ND-C4D-CHA-C1A
3	B	402	BLA	C3D-C4D-CHA-C1A
3	B	402	BLA	C1A-C2A-CAA-CBA
3	B	402	BLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	402	BLA	NA-C4A-CHB-C1B
3	B	402	BLA	C3A-C4A-CHB-C1B
3	B	402	BLA	NB-C1B-CHB-C4A
3	B	402	BLA	C2B-C1B-CHB-C4A
3	B	402	BLA	C2D-C3D-CAD-CBD
3	B	402	BLA	C4D-C3D-CAD-CBD
3	A	403	BLA	NA-C4A-CHB-C1B
3	A	403	BLA	C3A-C4A-CHB-C1B
3	C	403	BLA	NA-C1A-CHA-C4D
3	C	403	BLA	C2A-C1A-CHA-C4D
3	D	403	BLA	NA-C4A-CHB-C1B
3	D	403	BLA	C3A-C4A-CHB-C1B
2	B	401	NAP	O4B-C4B-C5B-O5B
2	D	401	NAP	O4B-C4B-C5B-O5B
2	A	401	NAP	C1B-C2B-O2B-P2B
3	C	403	BLA	NC-C4C-CHD-C1D
2	B	401	NAP	C3B-C2B-O2B-P2B
3	A	403	BLA	NC-C4C-CHD-C1D
3	C	403	BLA	C3C-C4C-CHD-C1D
2	B	401	NAP	C3D-C4D-C5D-O5D
2	A	401	NAP	C3D-C4D-C5D-O5D
2	C	401	NAP	C3D-C4D-C5D-O5D
2	D	401	NAP	C3D-C4D-C5D-O5D
3	B	402	BLA	C4C-C3C-CAC-CBC
3	D	403	BLA	C4C-C3C-CAC-CBC
3	A	403	BLA	ND-C4D-CHA-C1A
3	C	403	BLA	ND-C4D-CHA-C1A
2	B	401	NAP	C5D-O5D-PN-O3
2	A	401	NAP	C5D-O5D-PN-O3
2	C	401	NAP	C5B-O5B-PA-O3
2	C	401	NAP	C5D-O5D-PN-O3
2	D	401	NAP	C5D-O5D-PN-O3
2	C	401	NAP	PA-O3-PN-O2N
3	A	403	BLA	C3C-C4C-CHD-C1D
2	B	401	NAP	C5D-O5D-PN-O1N
2	A	401	NAP	C5D-O5D-PN-O1N
2	D	401	NAP	C5D-O5D-PN-O1N
2	A	401	NAP	O4B-C4B-C5B-O5B
3	D	402	BLA	ND-C4D-CHA-C1A
2	B	401	NAP	C1B-C2B-O2B-P2B
2	A	401	NAP	PA-O3-PN-O2N
2	D	401	NAP	PA-O3-PN-O2N

Continued on next page...

Continued from previous page...

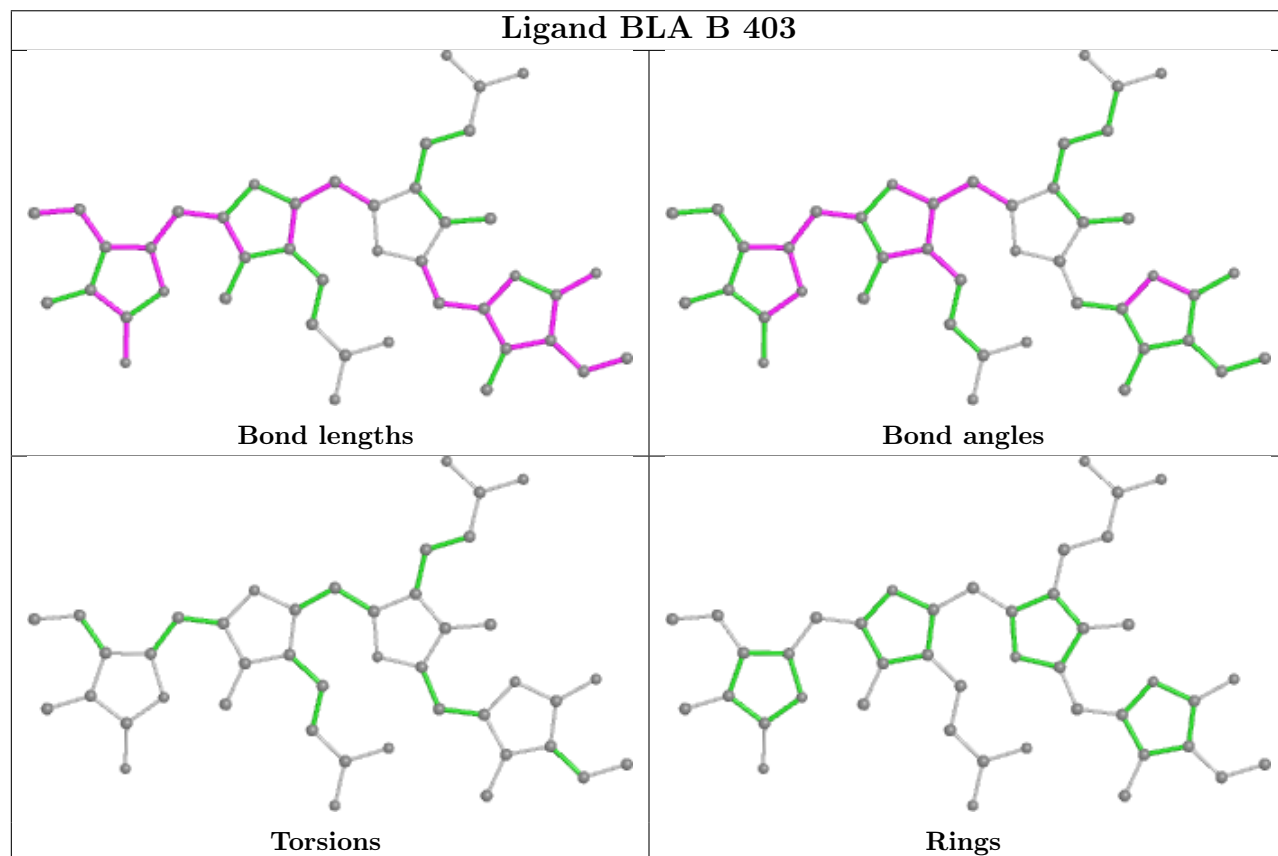
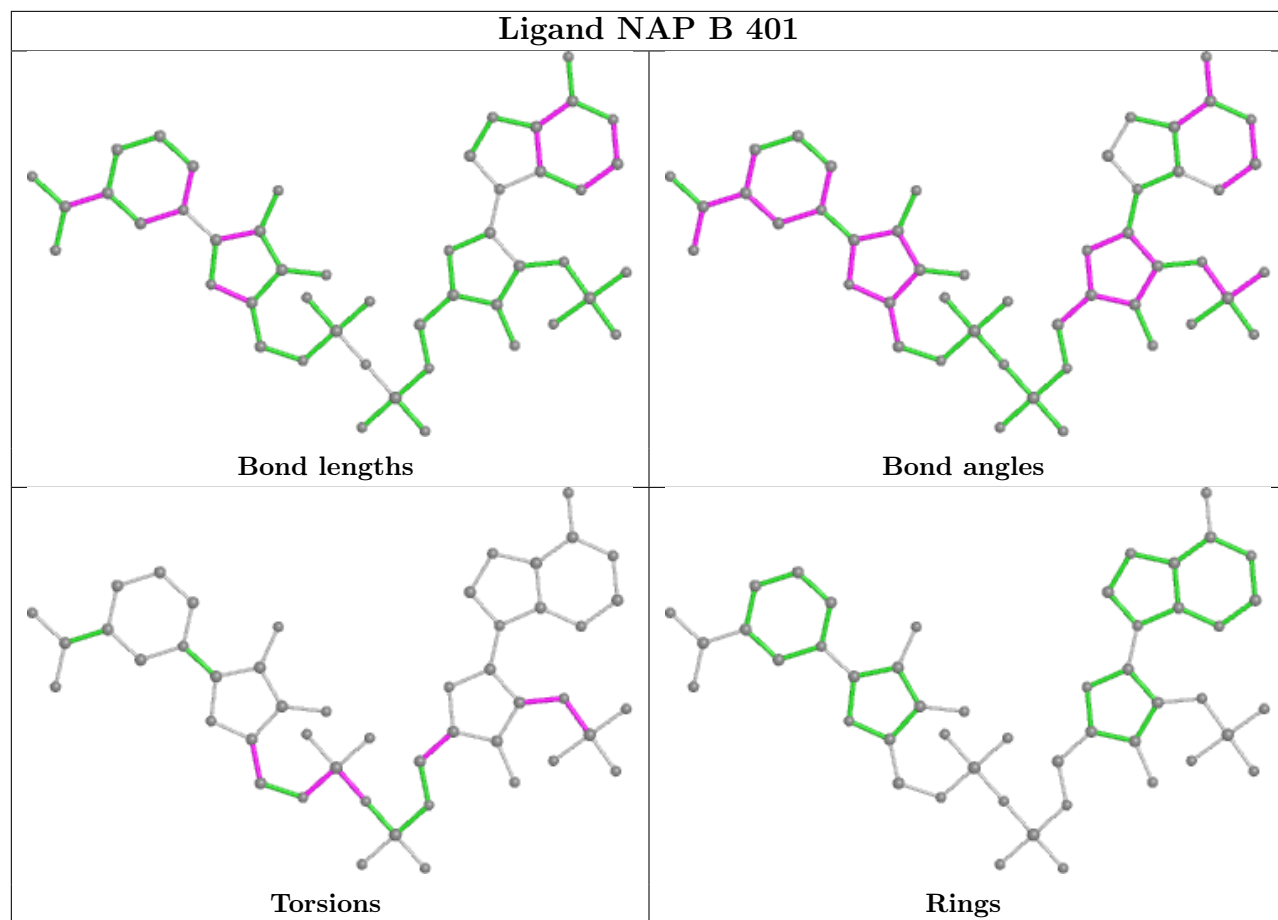
Mol	Chain	Res	Type	Atoms
2	C	401	NAP	PA-O3-PN-O1N
3	D	403	BLA	ND-C1D-CHD-C4C
2	C	401	NAP	C3B-C2B-O2B-P2B
2	A	401	NAP	C2B-O2B-P2B-O2X
2	D	401	NAP	C2B-O2B-P2B-O2X
2	B	401	NAP	PA-O3-PN-O2N
3	D	403	BLA	NC-C4C-CHD-C1D

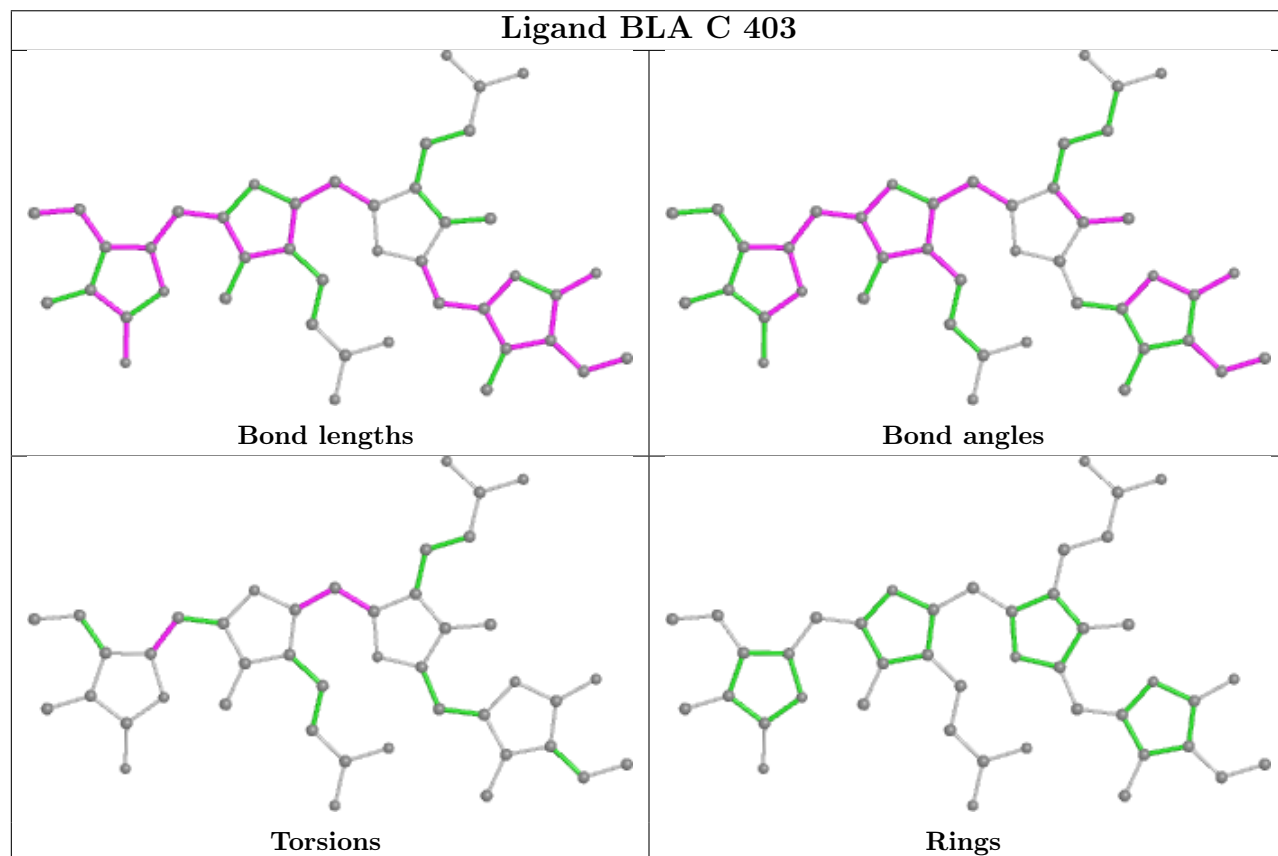
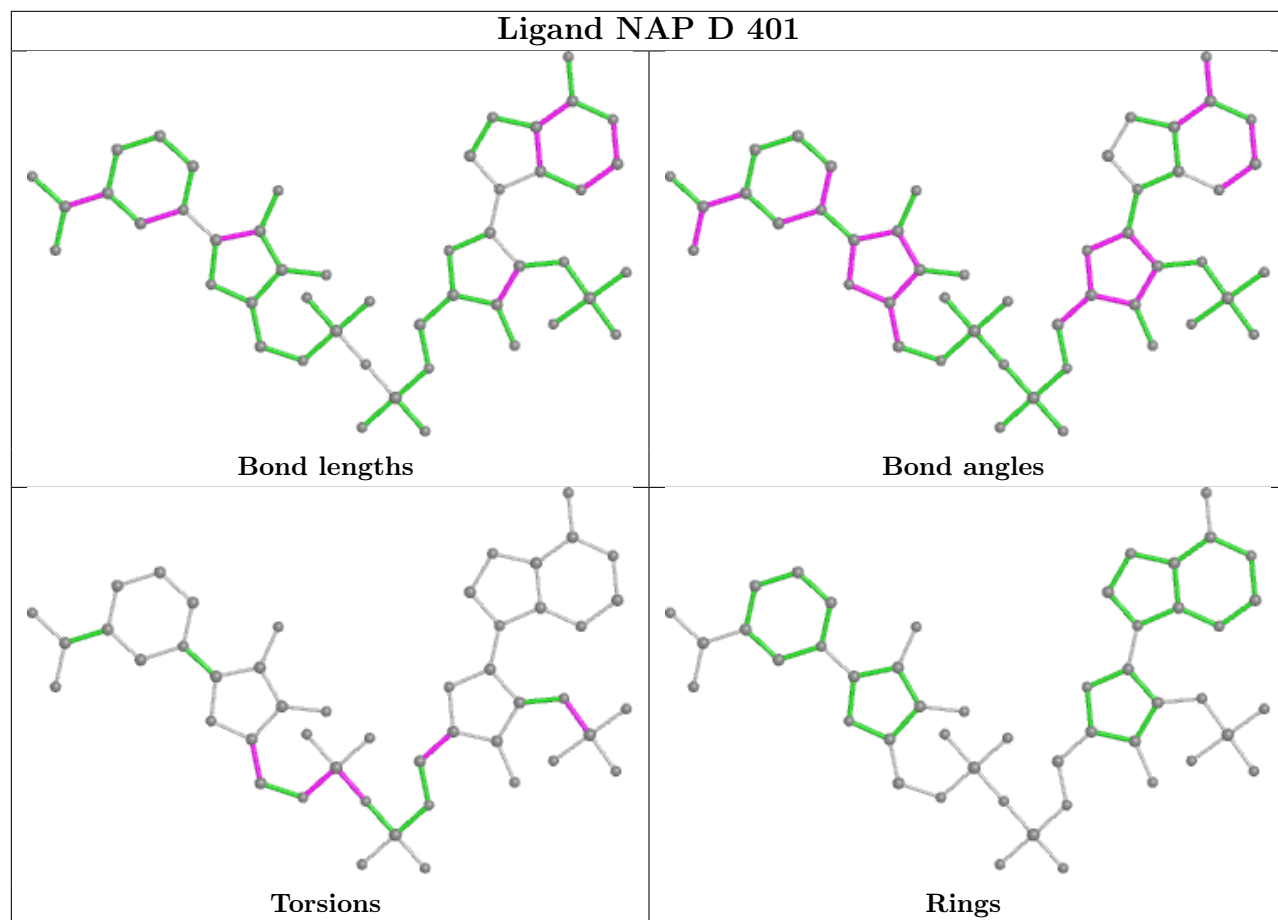
There are no ring outliers.

12 monomers are involved in 39 short contacts:

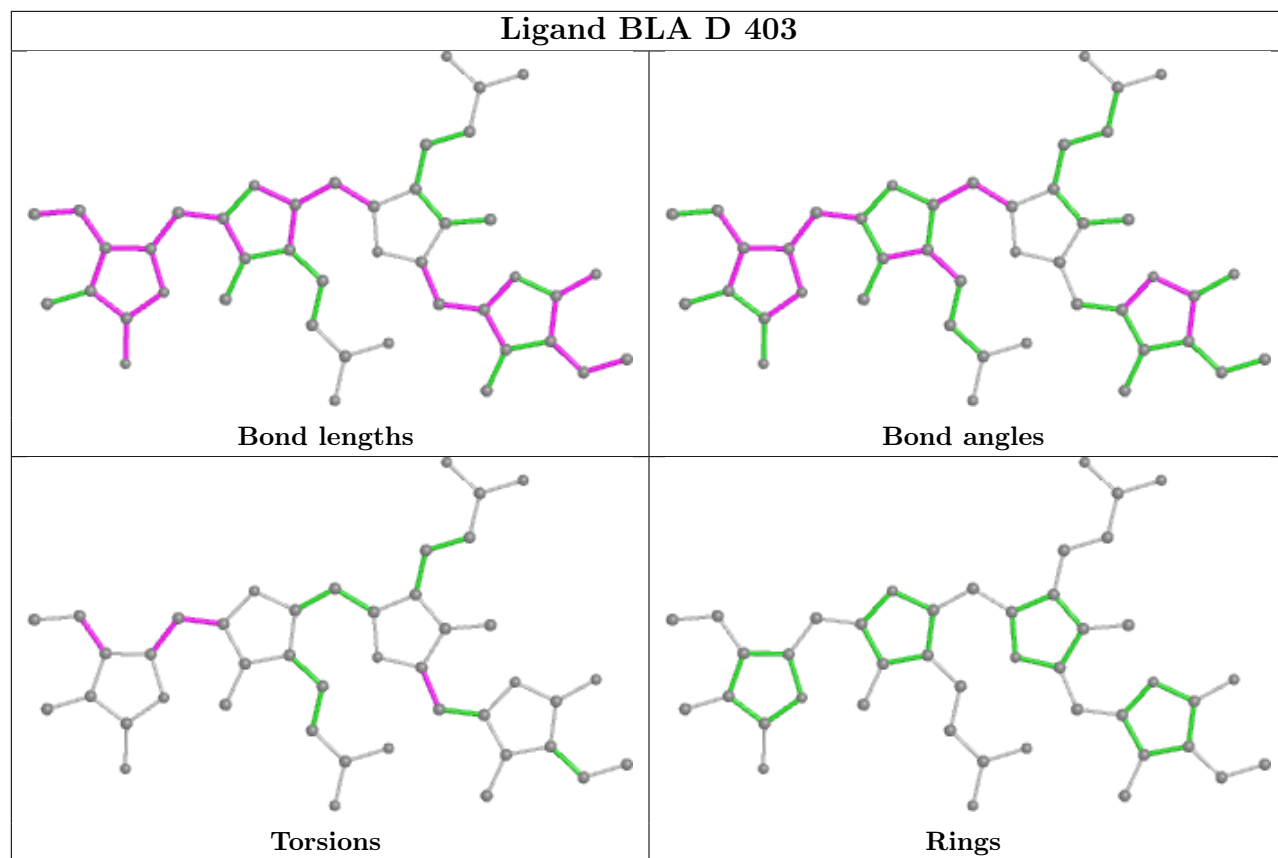
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NAP	1	0
3	B	403	BLA	4	0
2	D	401	NAP	1	0
3	C	403	BLA	6	0
3	D	403	BLA	5	0
3	B	402	BLA	8	0
2	C	401	NAP	3	0
3	D	402	BLA	4	0
3	A	402	BLA	4	0
3	A	403	BLA	3	0
3	C	402	BLA	5	0
2	A	401	NAP	3	0

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.

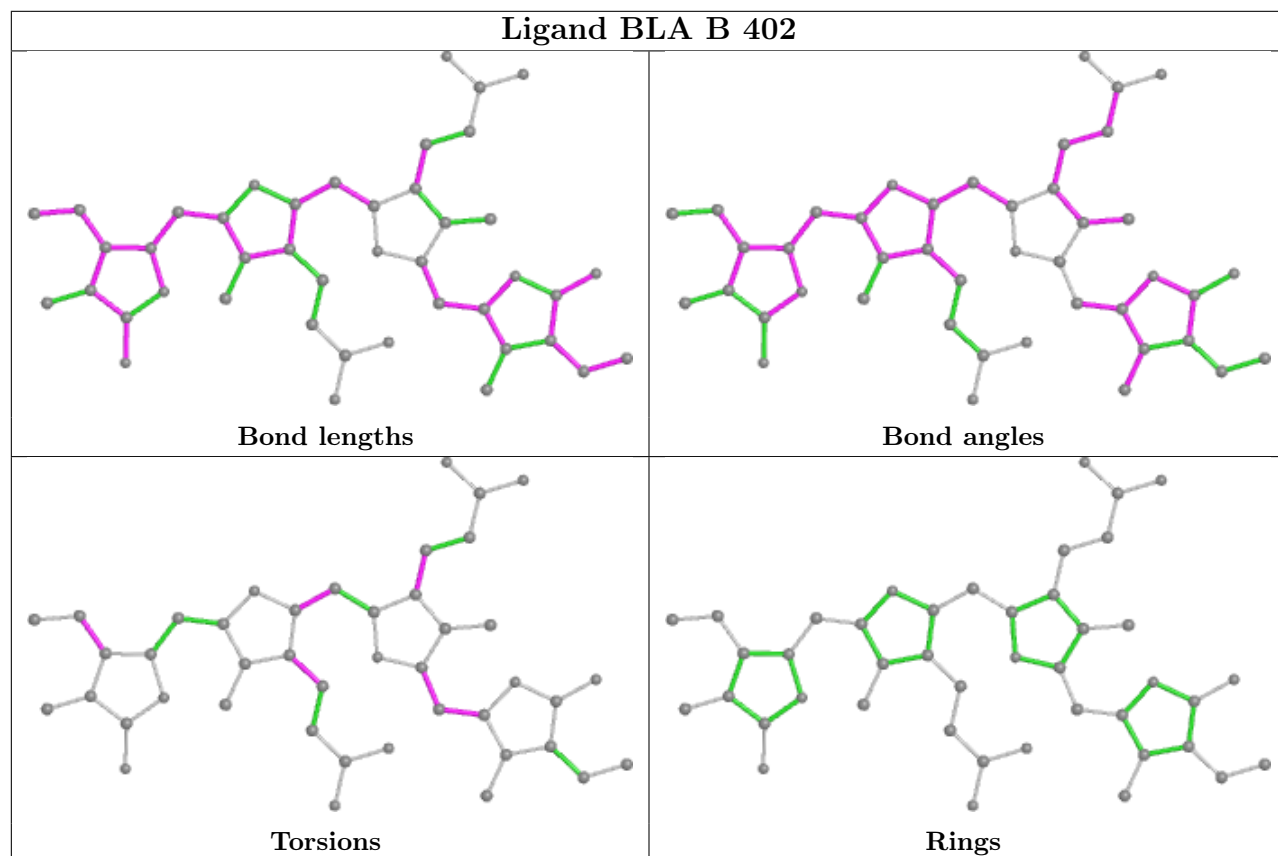




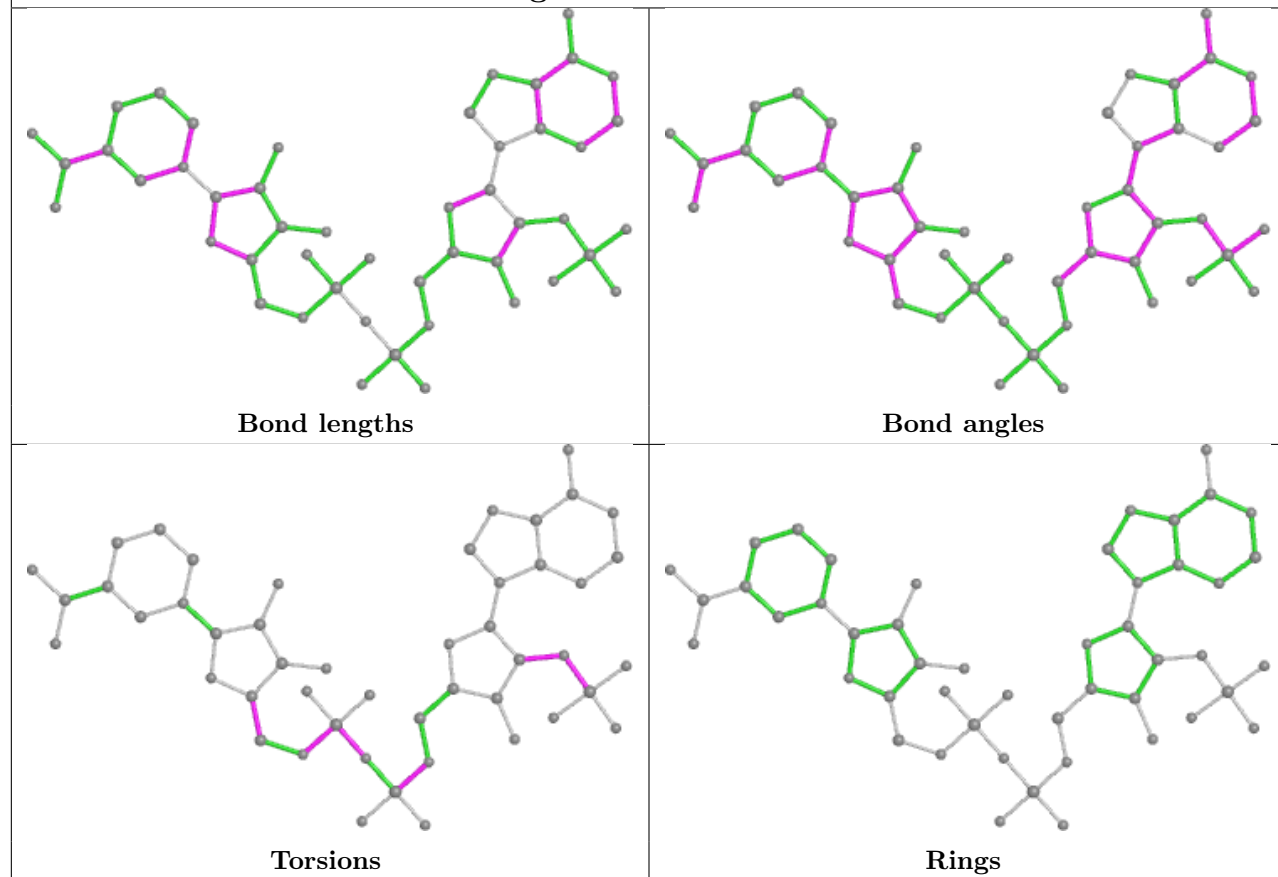
Ligand BLA D 403



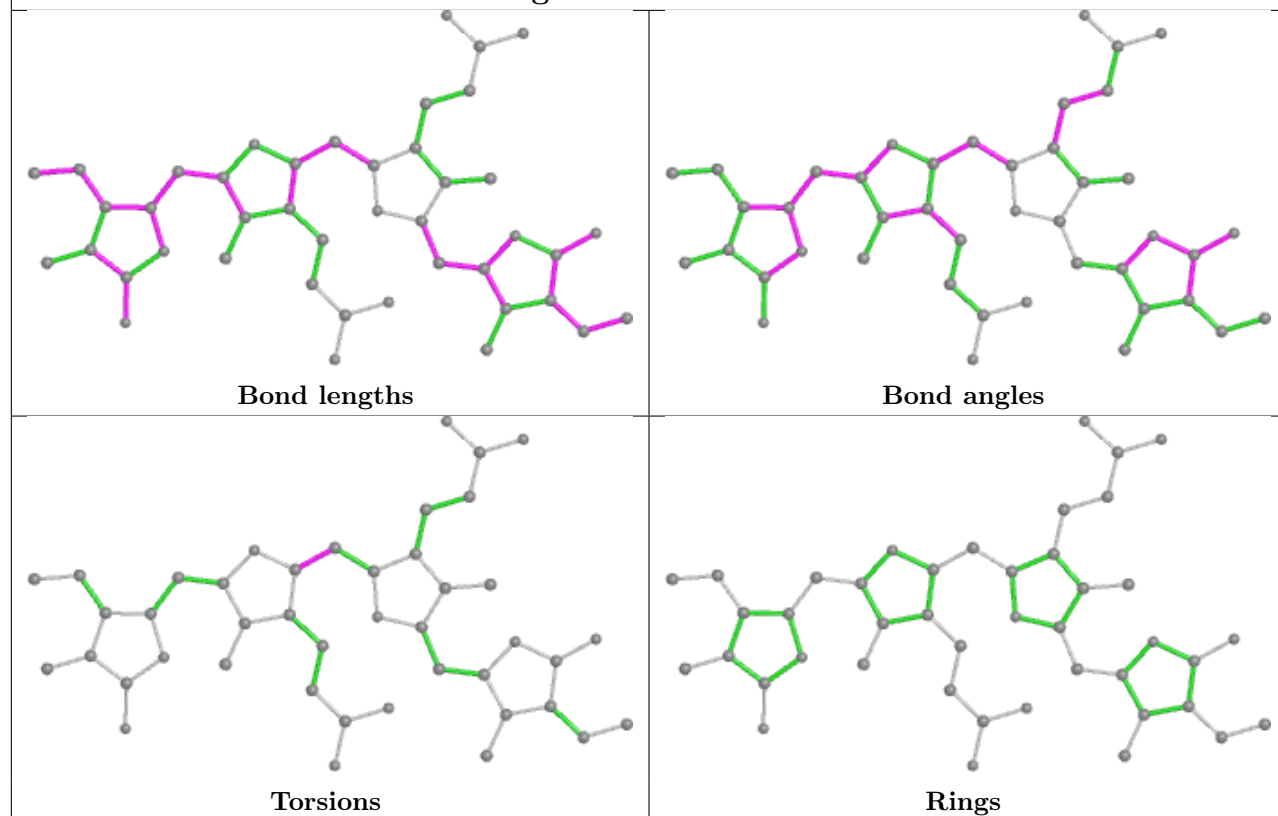
Ligand BLA B 402



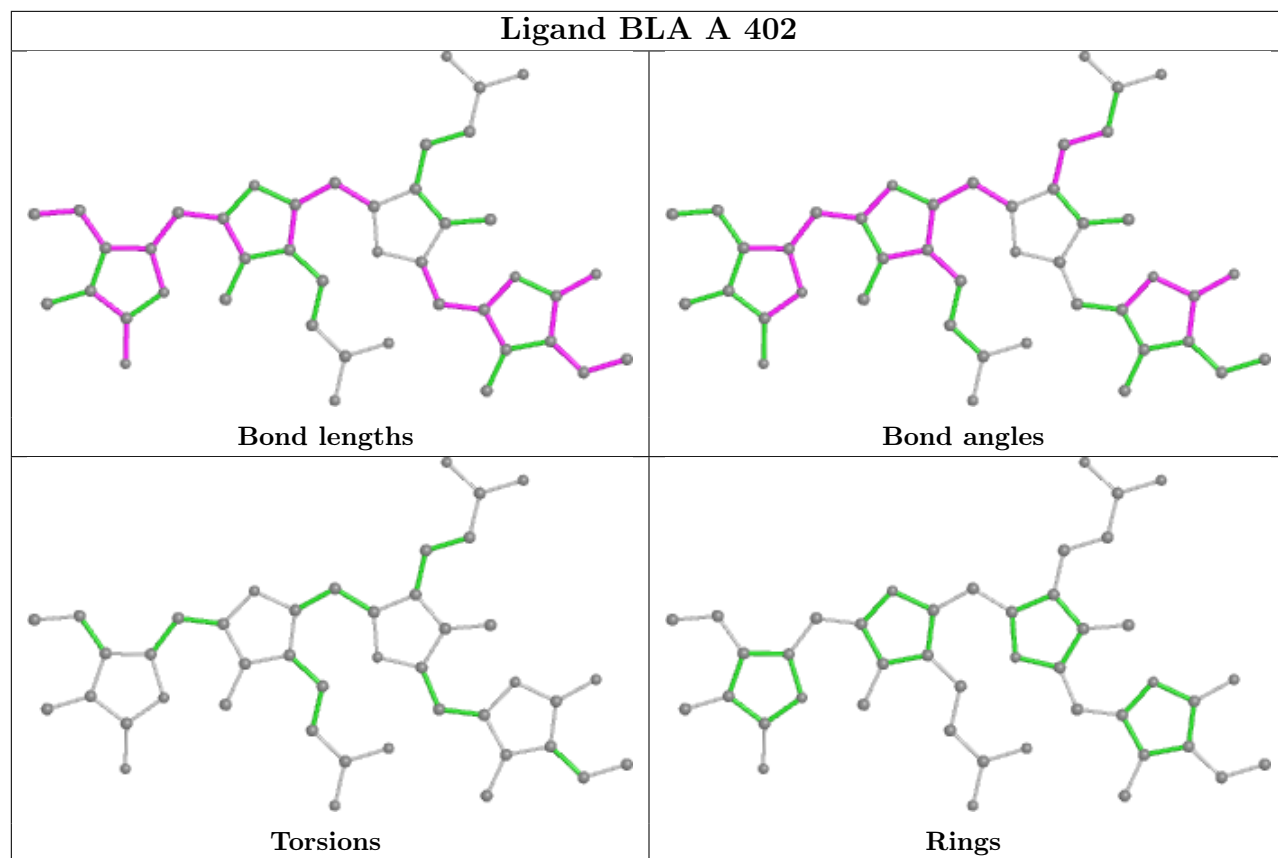
Ligand NAP C 401



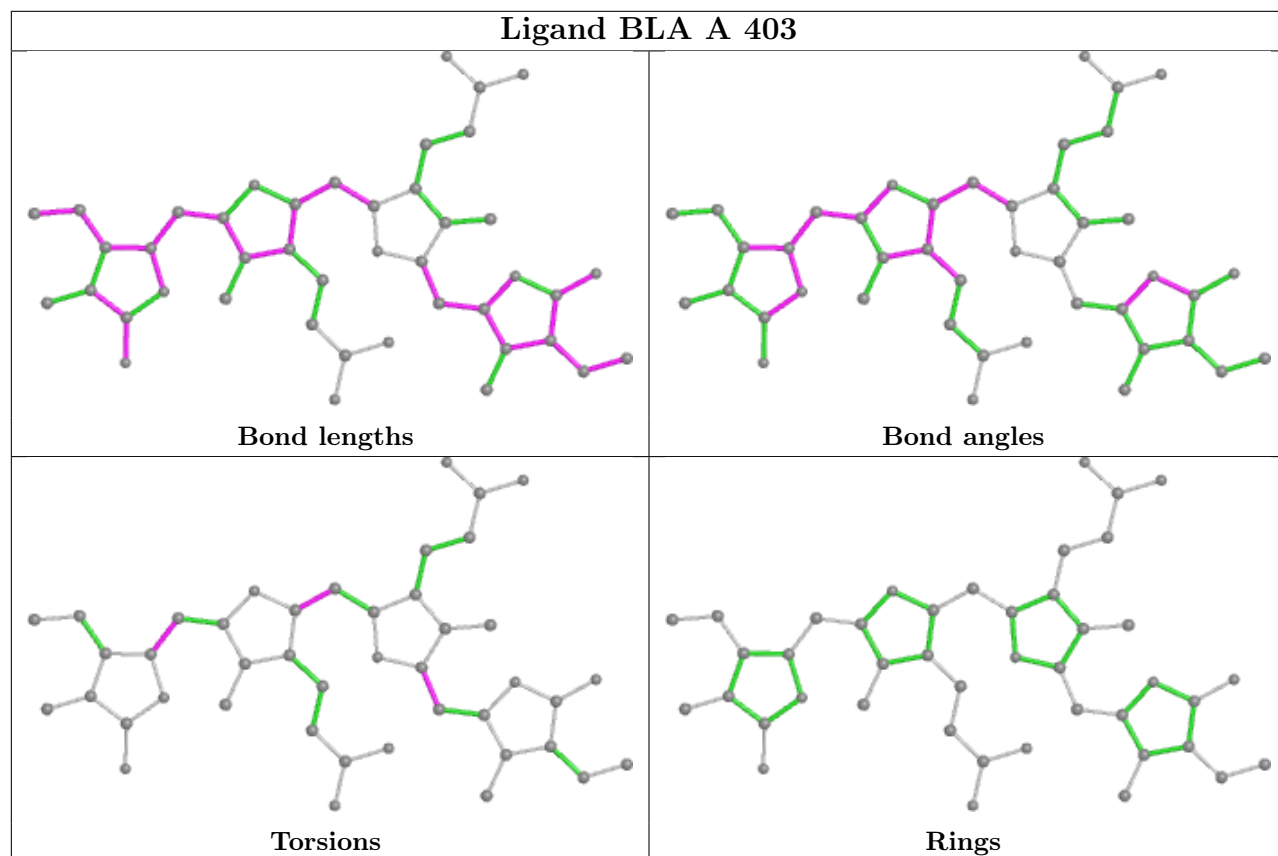
Ligand BLA D 402



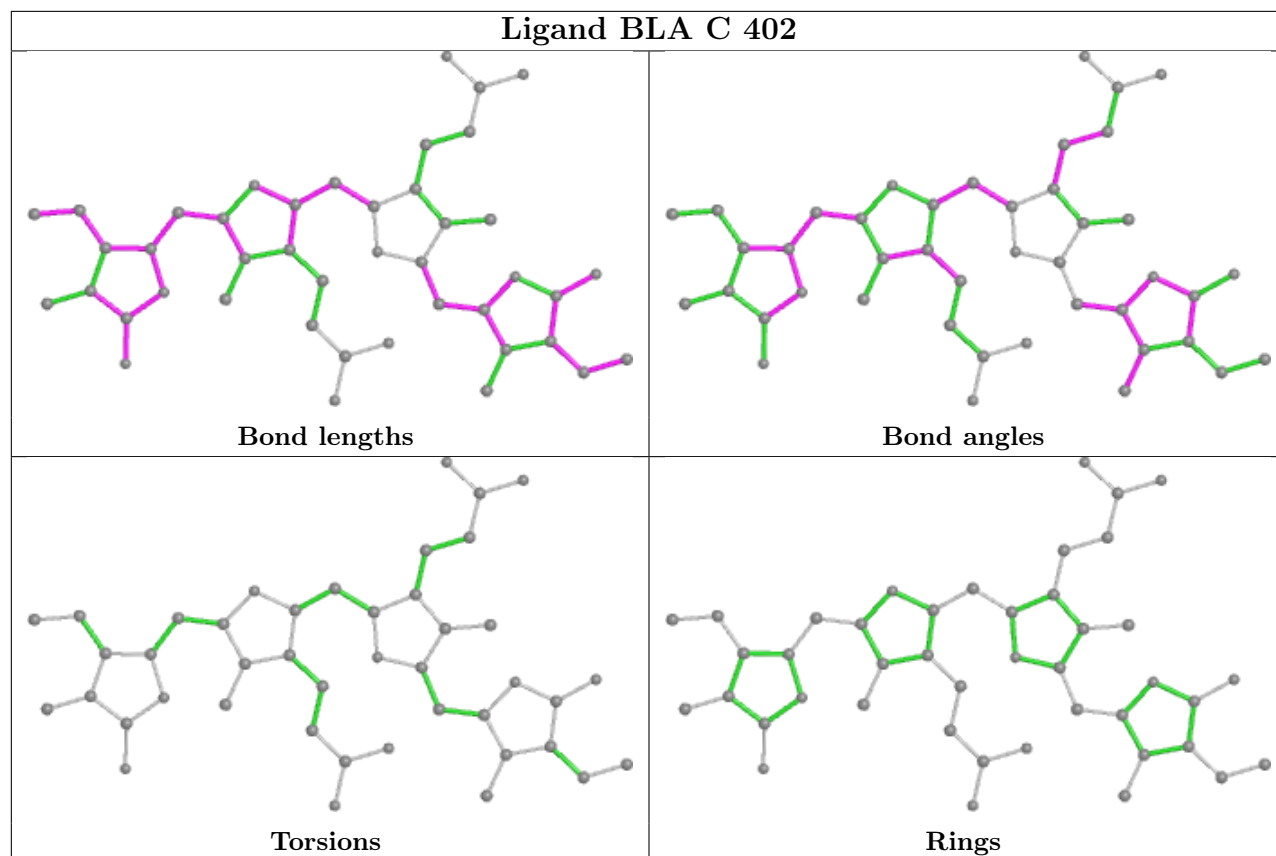
Ligand BLA A 402



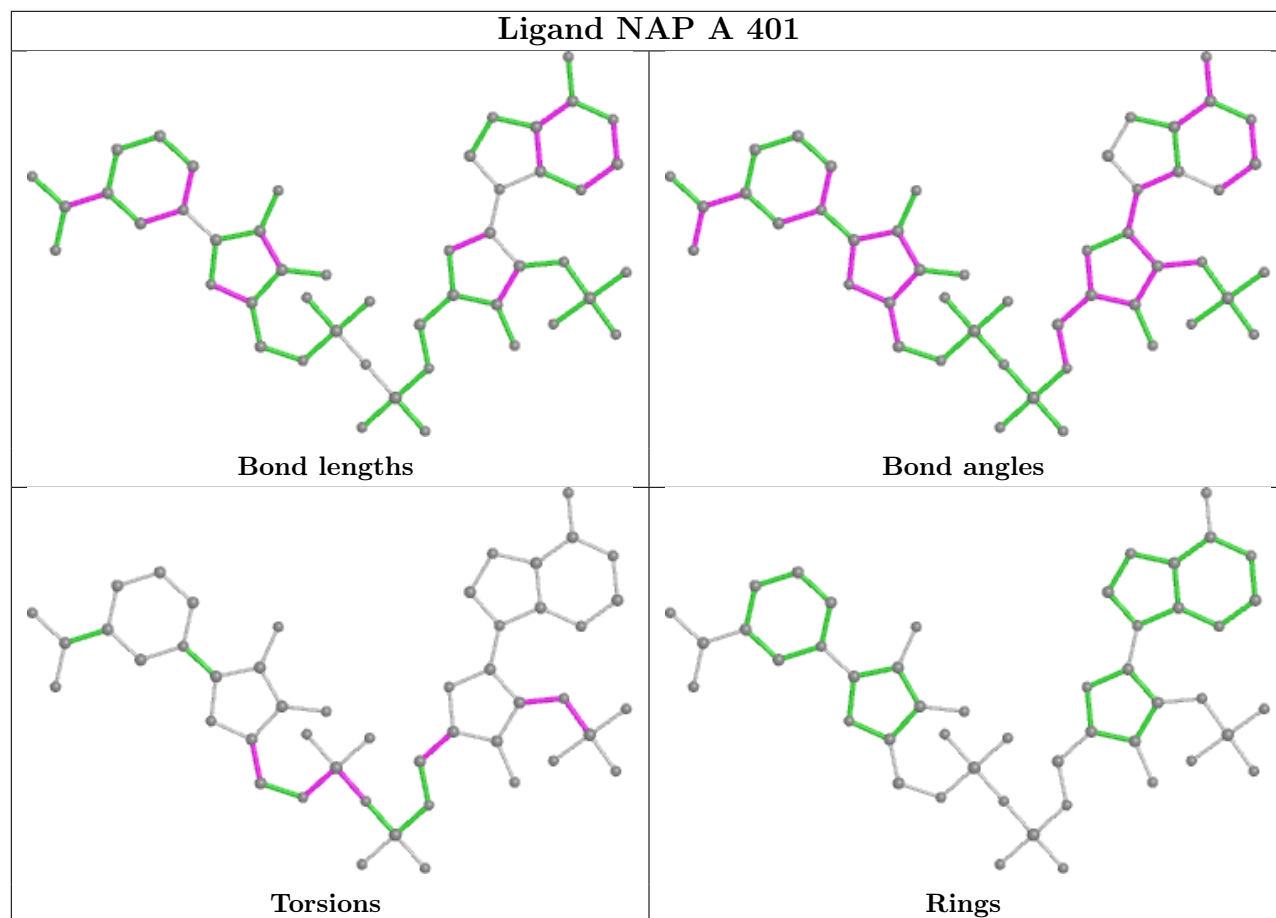
Ligand BLA A 403



Ligand BLA C 402



Ligand NAP A 401



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	317/331 (95%)	0.14	4 (1%) 77 73	15, 22, 36, 53	0
1	B	316/331 (95%)	0.24	8 (2%) 57 51	17, 24, 38, 79	0
1	C	316/331 (95%)	0.28	4 (1%) 77 73	20, 29, 41, 80	0
1	D	316/331 (95%)	0.37	7 (2%) 62 56	20, 27, 43, 59	0
All	All	1265/1324 (95%)	0.26	23 (1%) 68 64	15, 26, 41, 80	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	280	ARG	7.3
1	B	280	ARG	4.3
1	C	279	SER	4.2
1	D	271	THR	3.5
1	B	279	SER	3.3
1	D	270	GLN	3.0
1	D	9	THR	3.0
1	B	281	ARG	2.8
1	B	9	THR	2.8
1	D	246	ARG	2.8
1	A	9	THR	2.7
1	C	281	ARG	2.6
1	C	53	ASP	2.5
1	B	20	TYR	2.4
1	A	71	GLU	2.4
1	B	293	ASP	2.3
1	B	142	GLN	2.2
1	A	279	SER	2.2
1	B	324	TYR	2.1
1	D	67	ILE	2.1
1	D	116	GLN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	61	GLN	2.0
1	D	70	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 monosaccharides in this entry.

6.4 Ligands [i](#)

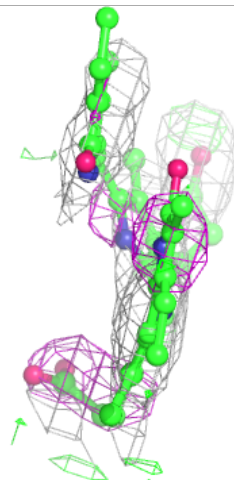
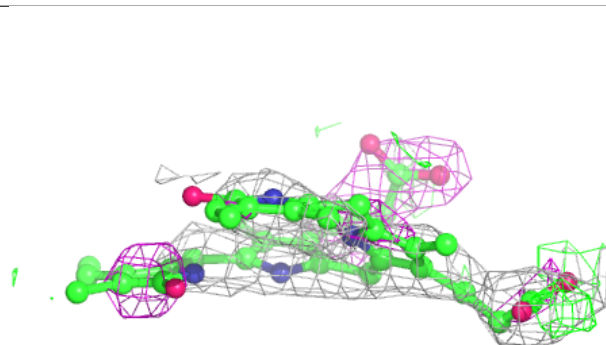
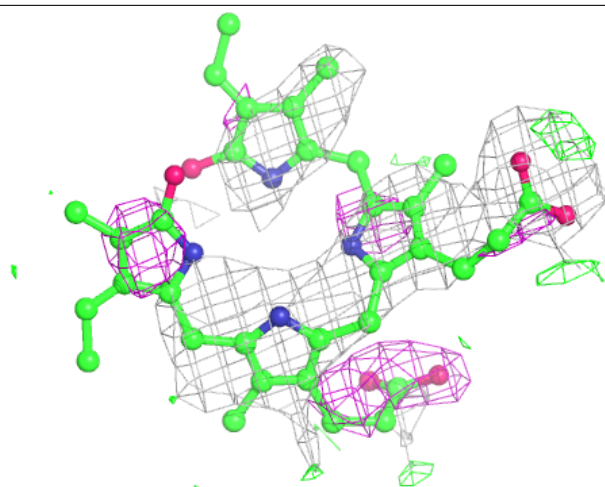
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BLA	B	402	43/43	0.59	0.54	35,55,75,81	0
3	BLA	C	403	43/43	0.62	0.49	33,63,80,83	0
3	BLA	C	402	43/43	0.83	0.23	31,47,61,65	0
3	BLA	B	403	43/43	0.87	0.21	25,40,53,59	0
3	BLA	A	403	43/43	0.88	0.21	19,25,31,34	0
3	BLA	D	403	43/43	0.88	0.21	23,29,32,38	0
2	NAP	C	401	48/48	0.89	0.20	29,31,36,40	0
2	NAP	A	401	48/48	0.91	0.18	18,21,27,29	0
3	BLA	D	402	43/43	0.92	0.17	22,25,27,29	0
3	BLA	A	402	43/43	0.92	0.17	17,21,24,26	0
2	NAP	B	401	48/48	0.94	0.16	22,25,30,34	0
2	NAP	D	401	48/48	0.95	0.15	22,23,29,31	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.

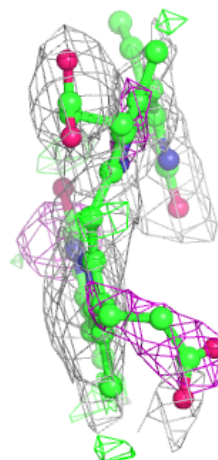
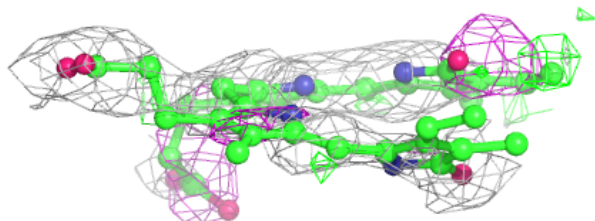
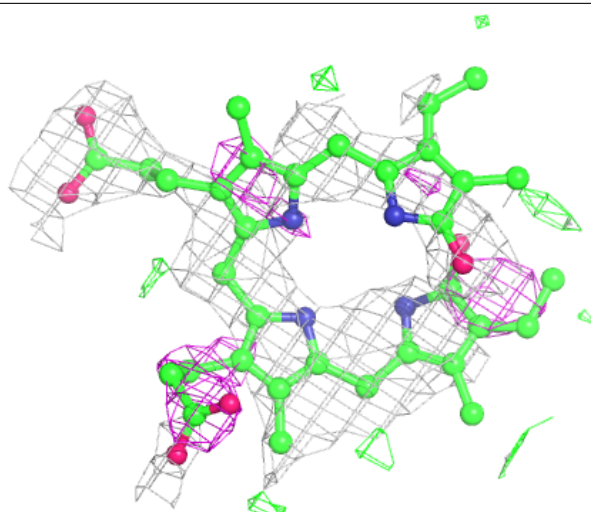
Electron density around BLA B 402:

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



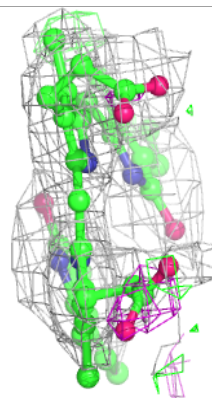
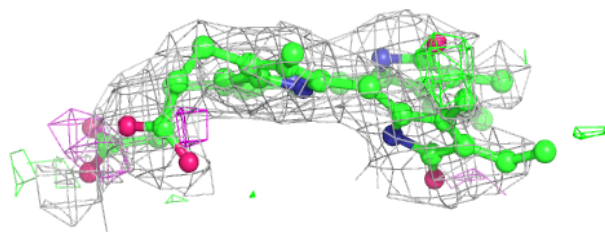
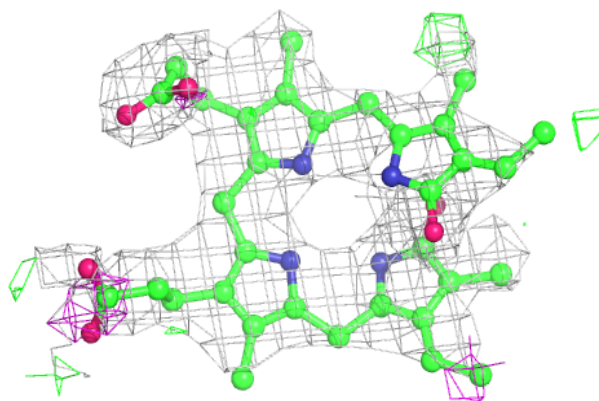
Electron density around BLA C 403:

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



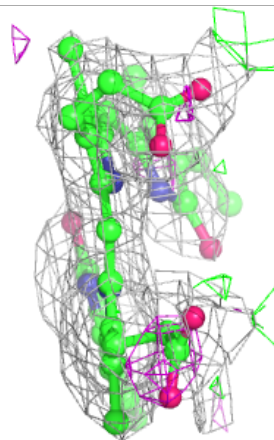
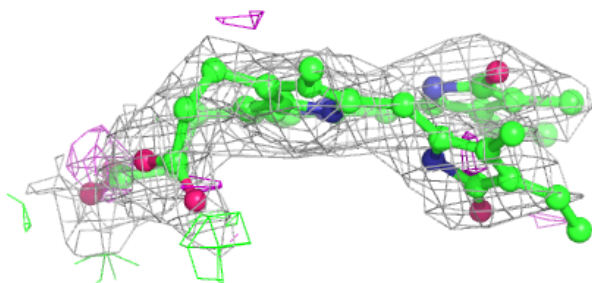
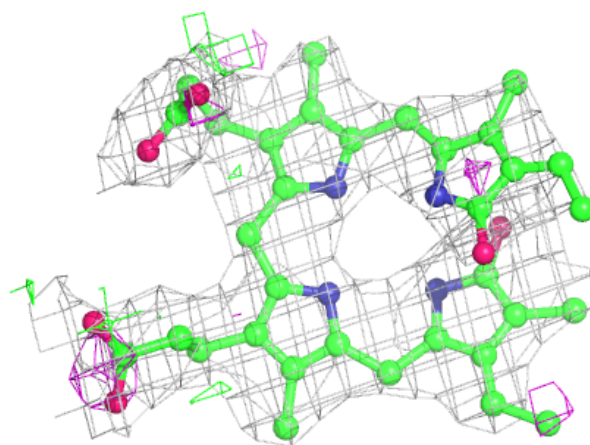
Electron density around BLA C 402:

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



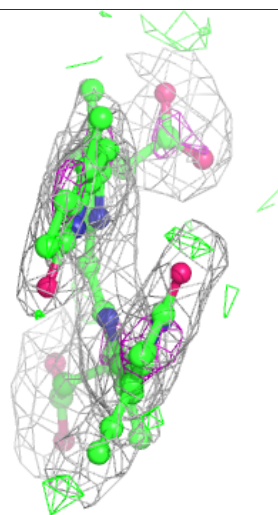
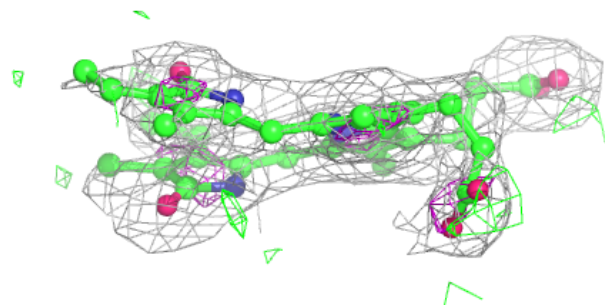
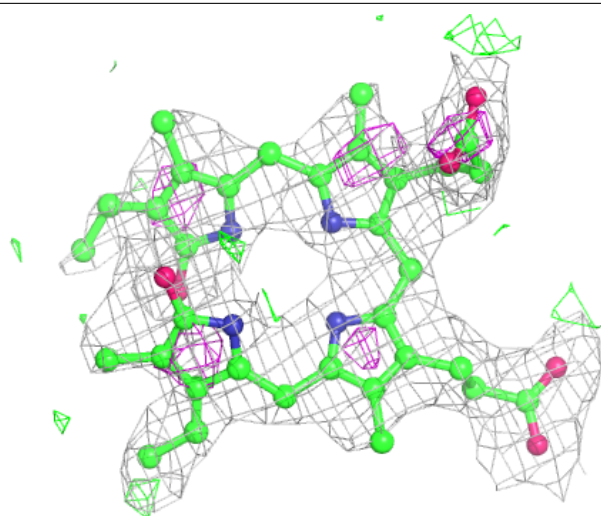
Electron density around BLA B 403:

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



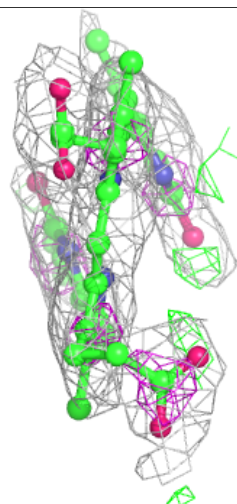
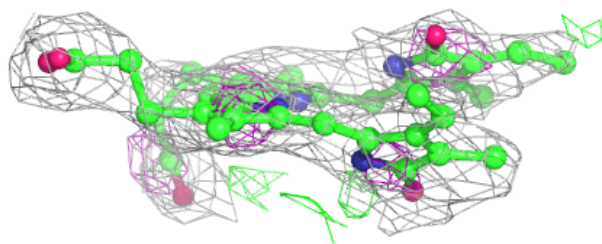
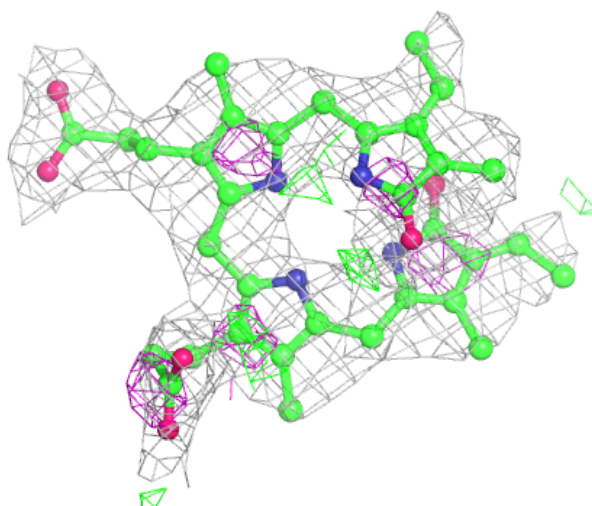
Electron density around BLA A 403:

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



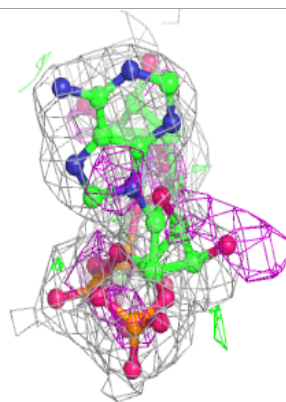
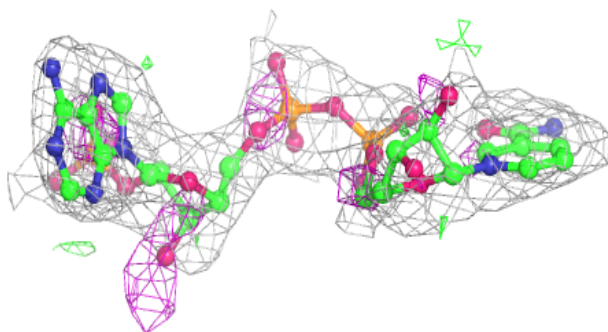
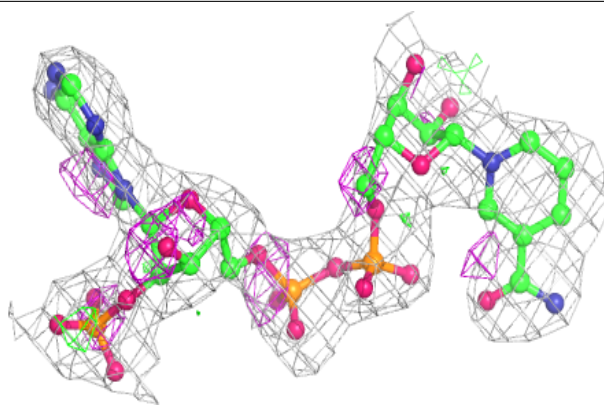
Electron density around BLA D 403:

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

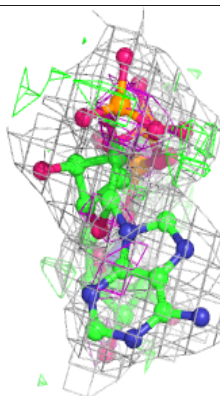
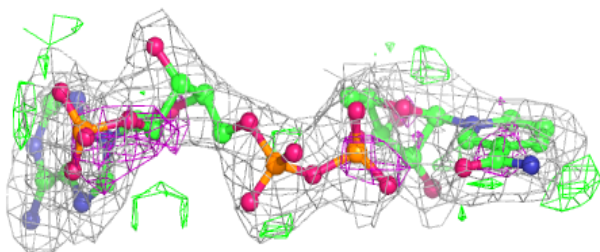
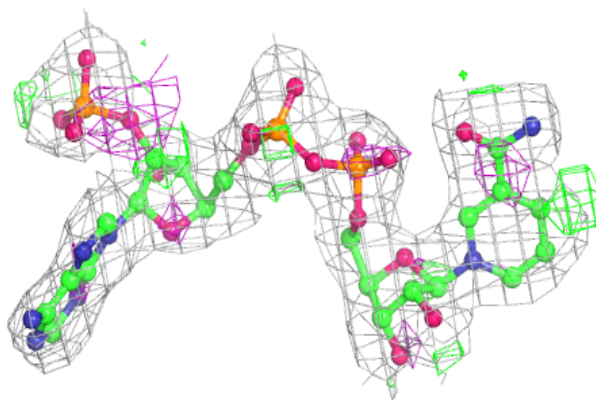


Electron density around NAP C 401:

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

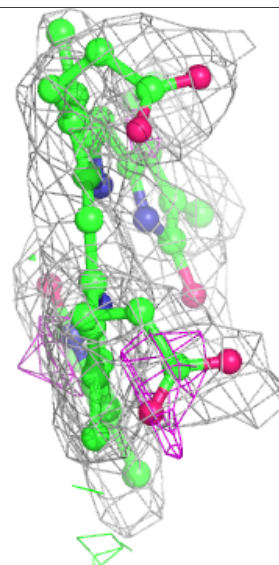
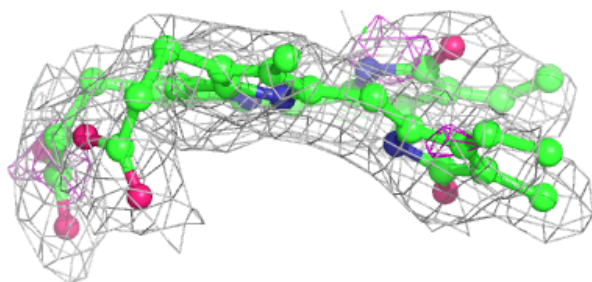
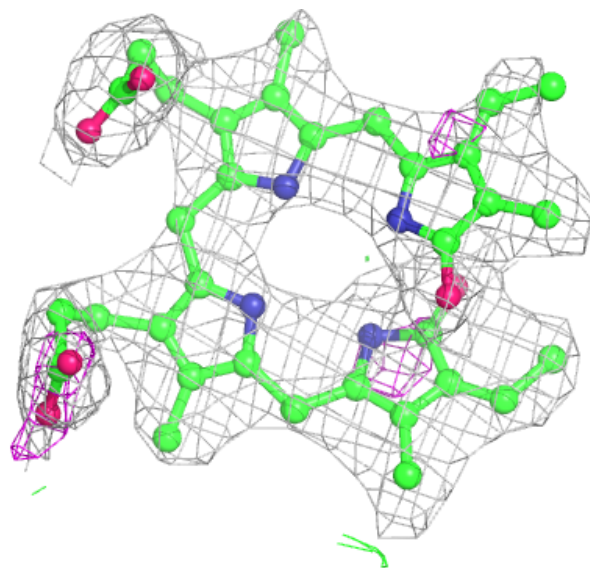
**Electron density around NAP A 401:**

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



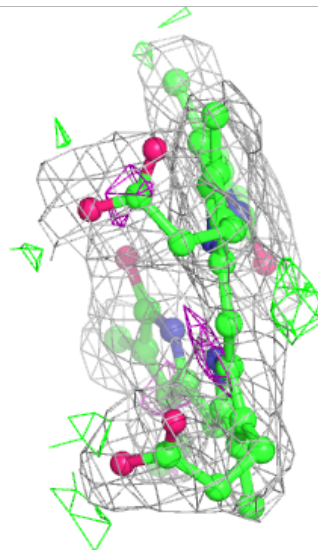
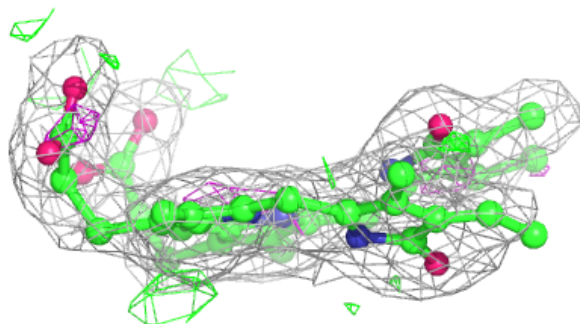
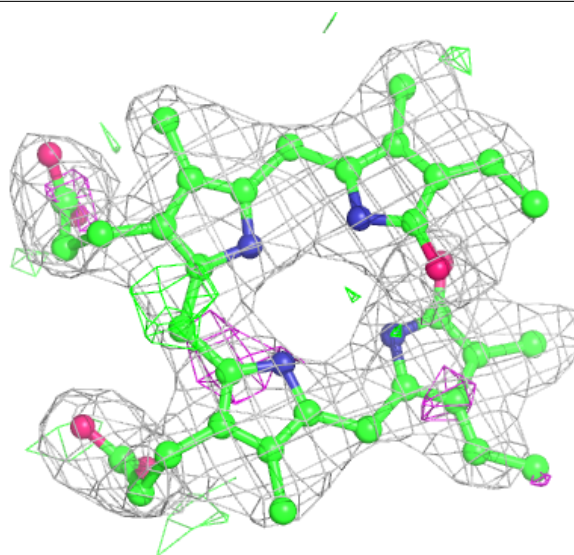
Electron density around BLA D 402:

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



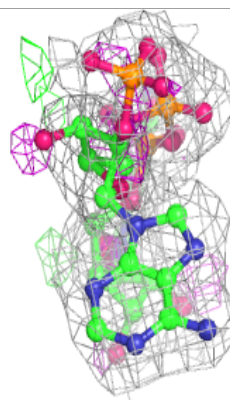
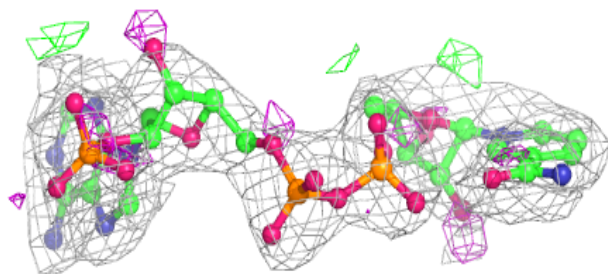
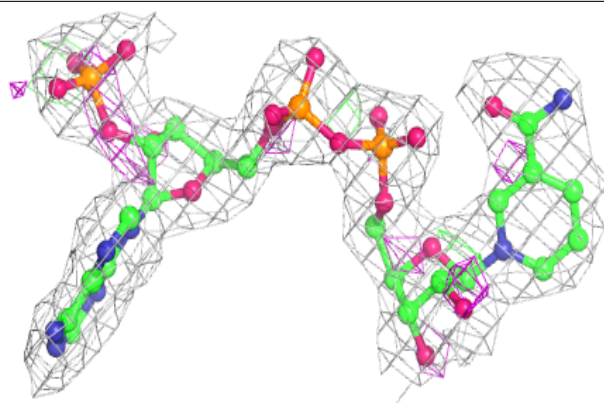
Electron density around BLA A 402:

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

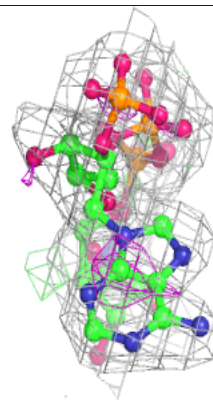
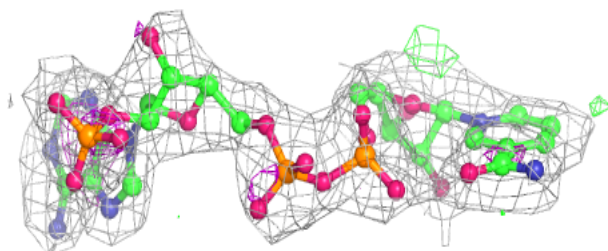
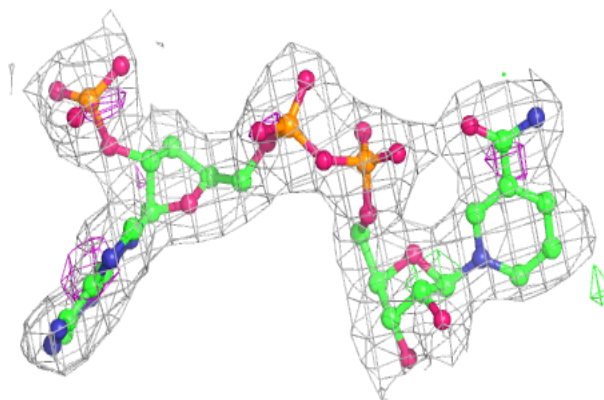


Electron density around NAP B 401:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.