



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 07:51 AM UTC

PDB ID : 8CFO / pdb_00008cfo
Title : Crystal structure of S-adenosyl-L-homocysteine hydrolase from *P. aeruginosa* in complex with F2X-Entry library fragment F04
Authors : Malecki, P.H.; Gawel, M.; Stepniewska, M.; Brzezinski, K.
Deposited on : 2023-02-03
Resolution : 2.13 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

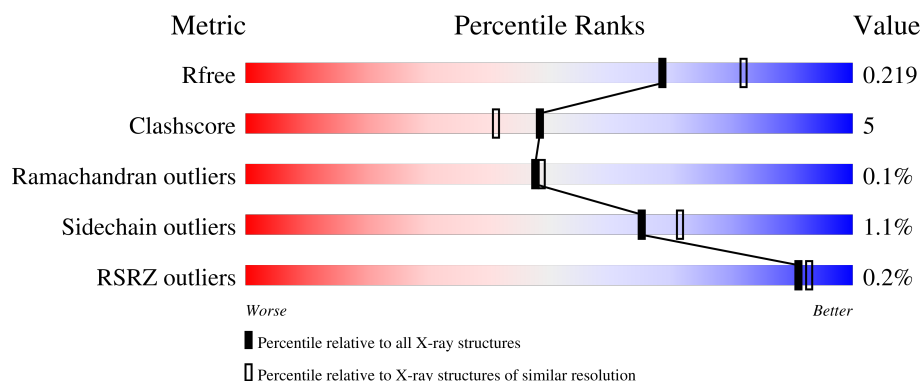
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	472	 86% 11% ..
1	B	472	 85% 13% .
1	C	472	 84% 13% ..
1	D	472	 87% 10% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16104 atoms, of which 128 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.

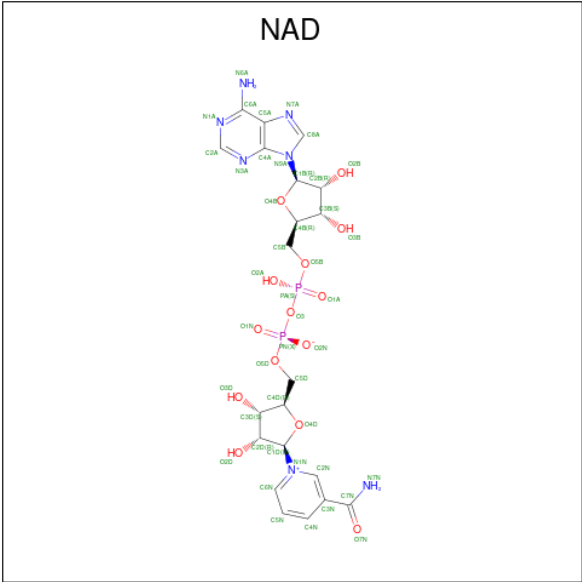
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	6	0
			3598	2268	623	684	23			
1	B	461	Total	C	N	O	S	0	4	0
			3577	2256	619	680	22			
1	C	462	Total	C	N	O	S	0	10	0
			3619	2283	626	687	23			
1	D	461	Total	C	N	O	S	0	5	0
			3582	2257	619	683	23			

There are 12 discrepancies between the modelled and reference sequences:

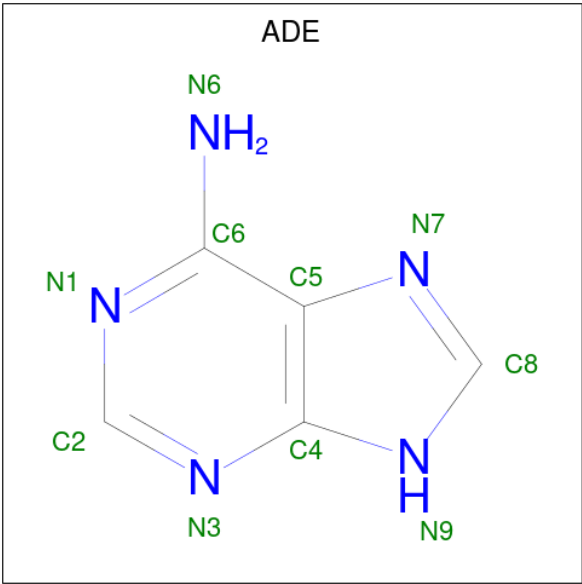
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9I685
A	-1	ASN	-	expression tag	UNP Q9I685
A	0	ALA	-	expression tag	UNP Q9I685
B	-2	SER	-	expression tag	UNP Q9I685
B	-1	ASN	-	expression tag	UNP Q9I685
B	0	ALA	-	expression tag	UNP Q9I685
C	-2	SER	-	expression tag	UNP Q9I685
C	-1	ASN	-	expression tag	UNP Q9I685
C	0	ALA	-	expression tag	UNP Q9I685
D	-2	SER	-	expression tag	UNP Q9I685
D	-1	ASN	-	expression tag	UNP Q9I685
D	0	ALA	-	expression tag	UNP Q9I685

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 3 is ADENINE (CCD ID: ADE) (formula: C₅H₅N₅).

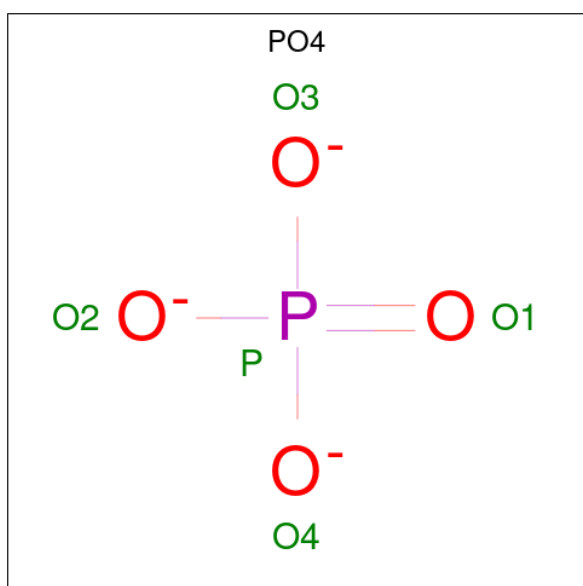


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	5	5		
3	B	1	Total	C	N	0	0
			10	5	5		
3	C	1	Total	C	N	0	0
			10	5	5		
3	D	1	Total	C	N	0	0
			10	5	5		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



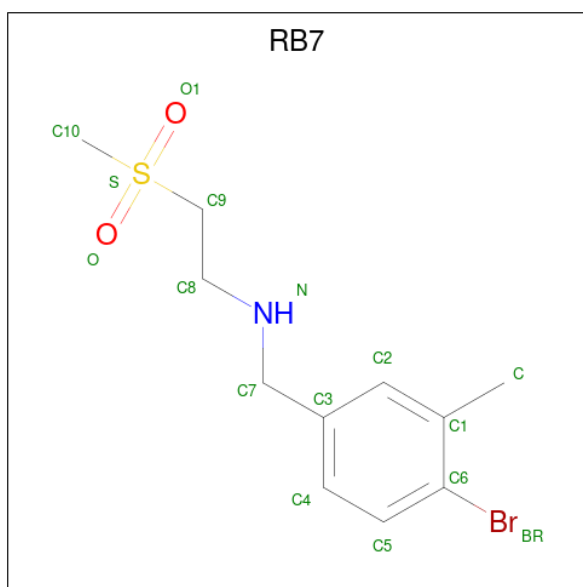
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		

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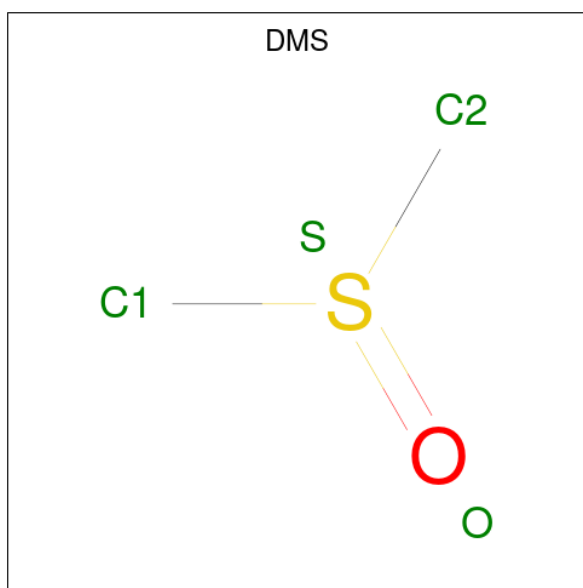
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total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

- Molecule 6 is N-[(4-bromo-3-methylphenyl)methyl]-2-(methylsulfonyl)ethan-1-amine (CCD ID: RB7) (formula: C₁₁H₁₆BrNO₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	A	1	Total 16	Br 1	C 11	N 1	O 2	S 1	0	0	
6	A	1	Total 16	Br 1	C 11	N 1	O 2	S 1	0	0	
6	A	1	Total 32	Br 1	C 11	H 16	N 1	O 2	S 1	0	0
6	A	1	Total 32	Br 1	C 11	H 16	N 1	O 2	S 1	0	0
6	A	1	Total 32	Br 1	C 11	H 16	N 1	O 2	S 1	0	0
6	B	1	Total 32	Br 1	C 11	H 16	N 1	O 2	S 1	0	0
6	B	1	Total 32	Br 1	C 11	H 16	N 1	O 2	S 1	0	0
6	C	1	Total 16	Br 1	C 11	N 1	O 2	S 1	0	0	
6	C	1	Total 16	Br 1	C 11	N 1	O 2	S 1	0	0	
6	C	1	Total 32	Br 1	C 11	H 16	N 1	O 2	S 1	0	0
6	C	1	Total 32	Br 1	C 11	H 16	N 1	O 2	S 1	0	0
6	D	1	Total 16	Br 1	C 11	N 1	O 2	S 1	0	0	
6	D	1	Total 16	Br 1	C 11	N 1	O 2	S 1	0	0	
6	D	1	Total 32	Br 1	C 11	H 16	N 1	O 2	S 1	0	0

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	O	S	0	0
			4	2	1	1		
7	D	1	Total	C	O	S	0	0
			4	2	1	1		

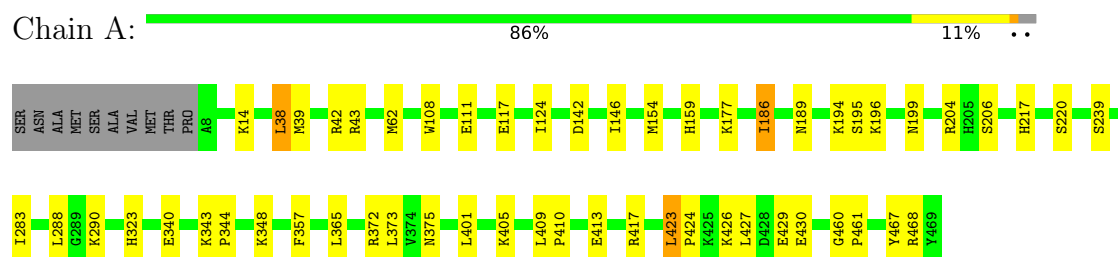
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	279	Total	O	0	5
			283	283		
8	B	248	Total	O	0	7
			251	251		
8	C	247	Total	O	0	4
			248	248		
8	D	288	Total	O	0	5
			291	291		

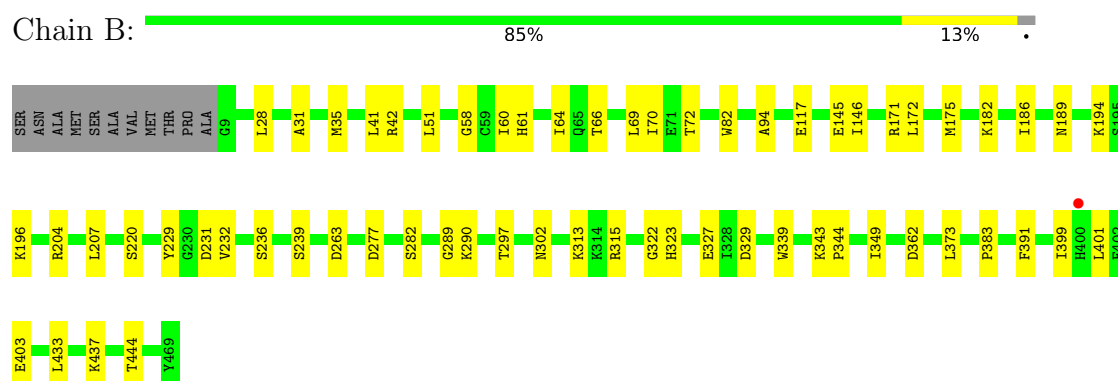
3 Residue-property plots [i](#)

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.

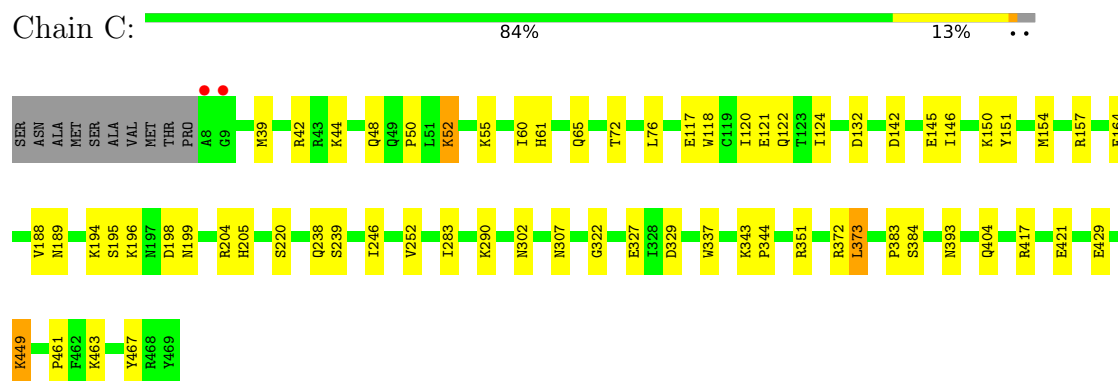
- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase

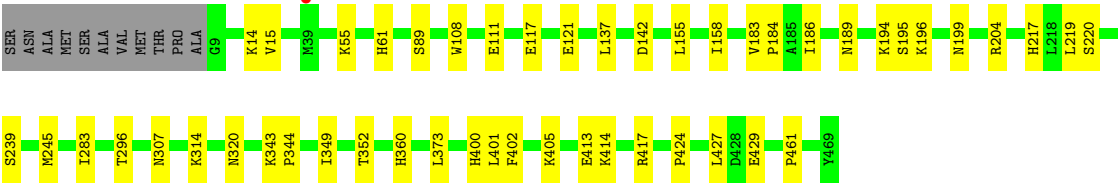


- Molecule 1: Adenosylhomocysteinase

Chain D:

87%

10%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.76Å 105.29Å 107.71Å 90.00° 99.72° 90.00°	Depositor
Resolution (Å)	34.92 – 2.13 34.92 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.92-2.13) 99.7 (34.92-2.13)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.19.2-4158	Depositor
R, R_{free}	0.171 , 0.219 0.171 , 0.219	Depositor DCC
R_{free} test set	2100 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16104	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: PO4, NAD, DMS, RB7, ADE, K

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	0/3673	0.56	0/4964
1	B	0.44	0/3649	0.55	0/4932
1	C	0.42	0/3706	0.55	0/5007
1	D	0.44	0/3651	0.55	0/4935
All	All	0.43	0/14679	0.55	0/19838

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	3598	0	3611	50	0
1	B	3577	0	3592	39	0
1	C	3619	0	3645	46	0
1	D	3582	0	3585	28	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0
3	A	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	20	0	0	1	0
5	B	10	0	0	0	0
5	C	25	0	0	2	0
5	D	20	0	0	1	0
6	A	80	48	0	5	0
6	B	32	32	0	3	0
6	C	64	32	0	3	0
6	D	48	16	0	2	0
7	C	4	0	6	0	0
7	D	4	0	6	0	0
8	A	283	0	0	1	0
8	B	251	0	0	2	0
8	C	248	0	0	5	0
8	D	291	0	0	5	0
All	All	15976	128	14565	161	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 5.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LEU:HD22	6:A:509:RB7:BR	2.27	0.90
1:B:146:ILE:HD11	6:B:506:RB7:BR	2.29	0.88
1:C:146:ILE:HD11	6:C:513:RB7:BR	2.31	0.85
1:C:120:ILE:HG21	1:C:146:ILE:HD12	1.63	0.80
1:C:189:ASN:HA	1:C:194:LYS:HD2	1.65	0.78
1:C:132:ASP:HB2	8:C:765:HOH:O	1.86	0.74
1:B:117:GLU:HB2	6:B:506:RB7:BR	2.41	0.74
1:D:189:ASN:HA	1:D:194:LYS:HD2	1.71	0.72
1:B:323:HIS:HA	1:B:373:LEU:HD21	1.71	0.71
1:D:117:GLU:O	1:D:121:GLU:HG2	1.93	0.69
1:A:283:ILE:HG23	1:A:288:LEU:HD12	1.77	0.66
1:A:290:LYS:HD2	8:A:668:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:SER:O	1:C:199:ASN:HB2	1.99	0.63
1:C:204[B]:ARG:HA	1:C:239:SER:HB2	1.79	0.63
1:C:204[A]:ARG:HA	1:C:239:SER:HB2	1.80	0.62
1:C:39[A]:MET:HA	1:C:39[A]:MET:HE2	1.82	0.62
1:A:186:ILE:HG13	1:A:401:LEU:HD11	1.82	0.62
1:C:39[A]:MET:HE1	1:C:42:ARG:CZ	2.31	0.61
1:D:314:LYS:HG3	5:D:505:PO4:O2	2.00	0.61
1:D:142:ASP:HB2	8:D:658:HOH:O	2.00	0.61
1:D:55:LYS:HE2	8:D:620:HOH:O	1.99	0.60
1:A:409:LEU:HD22	1:A:413:GLU:CB	2.32	0.60
1:B:189:ASN:HA	1:B:194:LYS:HD2	1.82	0.60
1:B:399:ILE:O	1:B:403:GLU:HG2	2.02	0.60
1:A:196:LYS:HD2	8:D:624:HOH:O	2.02	0.60
1:B:204:ARG:HA	1:B:239:SER:HB2	1.84	0.59
1:D:400:HIS:HB2	6:D:510:RB7:C7	2.33	0.58
1:C:157:ARG:HG3	8:C:683:HOH:O	2.03	0.58
1:A:39[A]:MET:HE1	1:A:42:ARG:CZ	2.33	0.58
1:A:409:LEU:HB3	1:A:413:GLU:HB2	1.86	0.58
1:B:322:GLY:O	1:B:373:LEU:HD23	2.05	0.57
1:C:118:TRP:O	1:C:122:GLN:HG2	2.04	0.57
1:B:145:GLU:OE1	1:B:171:ARG:NH2	2.37	0.57
5:C:505:PO4:O3	1:D:360:HIS:NE2	2.33	0.57
1:C:121[B]:GLU:OE2	1:C:150:LYS:NZ	2.36	0.56
1:C:205:HIS:CD2	1:C:383:PRO:HD3	2.41	0.56
1:A:189:ASN:HA	1:A:194:LYS:HD2	1.89	0.55
1:A:323:HIS:HA	1:A:373:LEU:HD21	1.89	0.55
1:A:124:ILE:HG23	1:A:154:MET:SD	2.47	0.55
1:A:283:ILE:CG2	1:A:288:LEU:HD12	2.37	0.55
1:B:315:ARG:NH1	1:B:362:ASP:HB2	2.20	0.55
1:D:186:ILE:HG13	1:D:401:LEU:HD11	1.89	0.55
1:C:146:ILE:CD1	6:C:513:RB7:BR	3.06	0.54
1:A:410:PRO:HD2	1:A:413:GLU:HG2	1.90	0.54
1:C:48[B]:GLN:HG3	1:C:50:PRO:HD3	1.88	0.54
1:A:204[B]:ARG:HA	1:A:239:SER:HB2	1.89	0.54
1:B:64:ILE:HD13	1:B:94:ALA:HB2	1.90	0.54
1:A:108:TRP:CE2	1:A:111:GLU:HG2	2.43	0.54
1:B:42:ARG:HG2	1:B:72:THR:HG23	1.91	0.53
1:C:48[B]:GLN:CG	1:C:50:PRO:HD3	2.38	0.53
1:C:121[B]:GLU:OE1	1:C:151:TYR:OH	2.22	0.53
1:A:142:ASP:O	1:A:146:ILE:HD12	2.08	0.53
1:C:429:GLU:OE1	1:C:461:PRO:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:THR:OG1	1:D:320:ASN:HB2	2.09	0.52
1:A:409:LEU:HD22	1:A:413:GLU:HB2	1.91	0.52
1:A:204[A]:ARG:HA	1:A:239:SER:HB2	1.91	0.52
1:C:204[B]:ARG:HD3	1:C:238[B]:GLN:OE1	2.09	0.51
1:C:117:GLU:HB3	6:C:513:RB7:BR	2.66	0.51
1:B:196[B]:LYS:HE2	1:B:231:ASP:OD2	2.11	0.51
1:B:186:ILE:HG12	1:B:401:LEU:HD11	1.93	0.50
1:C:373:LEU:HD22	2:C:501:NAD:N7N	2.27	0.50
1:D:204:ARG:HA	1:D:239:SER:HB2	1.93	0.50
1:A:117:GLU:HB2	6:A:510:RB7:BR	2.67	0.50
1:B:433:LEU:HG	1:B:437:LYS:HE3	1.93	0.50
1:A:186:ILE:HG13	1:A:401:LEU:CD1	2.41	0.50
1:B:28:LEU:HD23	1:B:64:ILE:HG23	1.94	0.50
1:D:413:GLU:OE1	1:D:417:ARG:NH1	2.42	0.50
1:A:410:PRO:HD2	1:A:413:GLU:CG	2.41	0.50
1:B:146:ILE:CD1	6:B:506:RB7:BR	3.09	0.49
1:A:14:LYS:HG3	1:A:108:TRP:CZ3	2.47	0.49
1:B:172:LEU:HA	1:B:175:MET:HE3	1.95	0.49
1:B:343:LYS:HB2	1:B:344:PRO:CD	2.43	0.49
1:C:351:ARG:NH2	5:C:509:PO4:O3	2.45	0.49
1:D:400:HIS:HB2	6:D:510:RB7:N	2.27	0.49
1:A:340:GLU:HG3	1:A:357:PHE:CZ	2.47	0.49
1:A:39[A]:MET:HE2	1:A:39[A]:MET:HA	1.94	0.48
1:A:108:TRP:CE2	6:A:512:RB7:C10	2.96	0.48
1:A:177:LYS:HE3	1:A:177:LYS:HB2	1.60	0.48
1:A:206:SER:HB2	1:A:375:ASN:HB2	1.94	0.48
1:B:277:ASP:OD1	1:B:282:SER:HB3	2.13	0.48
1:D:343:LYS:HB2	1:D:344:PRO:HD2	1.94	0.48
1:B:383:PRO:HA	8:B:626:HOH:O	2.14	0.48
1:C:283:ILE:HG13	1:C:307:ASN:HB3	1.96	0.48
1:A:426:LYS:O	1:A:430:GLU:HG3	2.14	0.47
1:C:290:LYS:HD2	8:C:798:HOH:O	2.14	0.47
1:C:302:ASN:OD1	1:C:329:ASP:HB2	2.15	0.47
1:A:195:SER:O	1:A:199:ASN:HB2	2.14	0.47
1:B:302:ASN:OD1	1:B:329:ASP:HB2	2.15	0.47
1:C:55:LYS:HD2	1:C:132:ASP:O	2.15	0.47
1:A:429:GLU:OE1	1:A:461:PRO:HA	2.15	0.46
1:B:66:THR:O	1:B:70:ILE:HG13	2.15	0.46
1:B:444:THR:O	1:C:252:VAL:HG12	2.14	0.46
1:C:60:ILE:O	1:C:61:HIS:C	2.58	0.46
1:B:290:LYS:HB3	1:B:290:LYS:HE3	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:VAL:HB	8:D:759:HOH:O	2.15	0.46
1:D:429:GLU:OE1	1:D:461:PRO:HA	2.15	0.46
1:B:182:LYS:HE2	1:B:182:LYS:HA	1.97	0.46
1:C:404:GLN:OE1	1:C:417:ARG:HD3	2.16	0.46
1:A:194:LYS:NZ	5:A:507:PO4:O2	2.49	0.45
1:D:14:LYS:HD2	1:D:14:LYS:HA	1.79	0.45
1:A:460:GLY:HA2	1:A:461:PRO:C	2.41	0.45
1:C:322:GLY:HA3	1:C:327:GLU:OE2	2.17	0.45
1:B:343:LYS:HB2	1:B:344:PRO:HD2	1.99	0.45
1:D:402:PHE:O	1:D:405:LYS:NZ	2.47	0.45
1:A:146:ILE:HD11	6:A:510:RB7:BR	2.72	0.44
1:A:38:LEU:HD12	1:A:38:LEU:HA	1.80	0.44
1:B:207:LEU:HD22	1:B:236:SER:HB3	1.99	0.44
1:C:65:GLN:HG3	1:C:384:SER:HA	1.99	0.44
1:D:137:LEU:C	1:D:137:LEU:HD23	2.42	0.44
1:A:159:HIS:ND1	1:A:405:LYS:HA	2.32	0.44
1:A:39[A]:MET:HE1	1:A:42:ARG:NE	2.32	0.44
1:C:44:LYS:O	1:C:44:LYS:HG2	2.18	0.44
1:C:337:TRP:CD1	1:C:351:ARG:HA	2.53	0.44
1:D:155:LEU:HA	1:D:158:ILE:HD12	2.00	0.44
1:A:468:ARG:HB2	1:D:196:LYS:HE3	1.99	0.44
1:A:39[B]:MET:O	1:A:43:ARG:HG3	2.17	0.44
1:C:72:THR:O	1:C:76:LEU:HG	2.18	0.43
1:C:124:ILE:HG23	1:C:154:MET:SD	2.58	0.43
1:C:343:LYS:HB2	1:C:344:PRO:HD2	1.99	0.43
1:B:58:GLY:HA3	1:B:82:TRP:CZ3	2.53	0.43
1:B:204:ARG:HD3	8:B:616:HOH:O	2.19	0.43
1:A:146:ILE:HD11	6:A:510:RB7:C5	2.49	0.43
1:C:421:GLU:HG3	8:C:778:HOH:O	2.18	0.43
1:A:62:MET:HE3	1:A:62:MET:C	2.44	0.43
1:D:219:LEU:O	1:D:245:MET:HG2	2.19	0.43
1:A:189:ASN:O	1:A:195:SER:HB3	2.18	0.42
1:A:424:PRO:HD2	1:A:427:LEU:HD12	2.01	0.42
1:D:283:ILE:HG13	1:D:307:ASN:HB3	2.01	0.42
1:A:343:LYS:HB2	1:A:344:PRO:HD2	2.02	0.42
1:B:41:LEU:HD23	1:B:41:LEU:HA	1.82	0.42
1:B:289:GLY:O	1:B:313:LYS:HB2	2.20	0.42
1:A:409:LEU:HD22	1:A:413:GLU:HB3	2.01	0.42
1:A:348:LYS:HA	1:A:365:LEU:O	2.20	0.41
1:C:463:LYS:HE2	1:C:467:TYR:CE2	2.55	0.41
1:B:339:TRP:CE2	1:B:349:ILE:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:O	1:A:373:LEU:C	2.62	0.41
1:A:417:ARG:HG3	1:A:417:ARG:O	2.19	0.41
1:D:424:PRO:HD2	1:D:427:LEU:HD12	2.02	0.41
1:C:142:ASP:O	1:C:146:ILE:HG13	2.20	0.41
1:C:164:GLU:O	1:C:164:GLU:HG3	2.19	0.41
1:D:108:TRP:O	1:D:111:GLU:HG3	2.20	0.41
1:B:322:GLY:HA3	1:B:327:GLU:OE2	2.20	0.41
1:D:414:LYS:NZ	8:D:616:HOH:O	2.53	0.41
1:A:290:LYS:HB3	1:A:290:LYS:HE3	1.78	0.41
1:C:449:LYS:HA	1:C:449:LYS:HD3	1.36	0.41
1:A:467:TYR:OH	2:D:501:NAD:O2A	2.28	0.41
1:D:183:VAL:HB	1:D:184:PRO:HD2	2.03	0.41
1:B:60:ILE:O	1:B:61:HIS:C	2.63	0.41
1:B:69:LEU:HB2	1:B:391:PHE:CD2	2.56	0.41
1:D:61:HIS:HD1	1:D:89:SER:CB	2.33	0.41
1:D:195:SER:O	1:D:199:ASN:HB2	2.21	0.41
1:A:413:GLU:HA	1:A:413:GLU:OE1	2.21	0.41
1:B:229:TYR:OH	1:B:263:ASP:OD2	2.30	0.41
1:C:52:LYS:HE2	1:C:52:LYS:HB2	1.69	0.41
1:C:142:ASP:HB2	8:C:688:HOH:O	2.20	0.40
1:C:188:VAL:HG13	1:C:393:ASN:HB3	2.03	0.40
1:C:372:ARG:O	1:C:373:LEU:C	2.64	0.40
1:B:51:LEU:HA	1:B:51:LEU:HD23	1.86	0.40
1:C:246:ILE:HD12	1:C:246:ILE:N	2.35	0.40
1:B:31:ALA:O	1:B:35:MET:HG3	2.21	0.40
1:B:232:VAL:HG12	1:B:297:THR:HB	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	466/472 (99%)	448 (96%)	18 (4%)	0	100	100
1	B	463/472 (98%)	450 (97%)	13 (3%)	0	100	100
1	C	470/472 (100%)	456 (97%)	13 (3%)	1 (0%)	43	42
1	D	464/472 (98%)	451 (97%)	13 (3%)	0	100	100
All	All	1863/1888 (99%)	1805 (97%)	57 (3%)	1 (0%)	48	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	373	LEU

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	383/385 (100%)	378 (99%)	5 (1%)	61	67
1	B	381/385 (99%)	380 (100%)	1 (0%)	86	90
1	C	387/385 (100%)	380 (98%)	7 (2%)	51	57
1	D	381/385 (99%)	376 (99%)	5 (1%)	61	67
All	All	1532/1540 (100%)	1514 (99%)	18 (1%)	65	69

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	186	ILE
1	A	217	HIS
1	A	220	SER
1	A	423	LEU
1	B	220	SER
1	C	52	LYS
1	C	145	GLU
1	C	196[A]	LYS
1	C	196[B]	LYS

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Mol	Chain	Res	Type
1	C	198	ASP
1	C	220	SER
1	C	449	LYS
1	D	217	HIS
1	D	220	SER
1	D	349	ILE
1	D	352	THR
1	D	373	LEU

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

Mol	Chain	Res	Type
1	A	197	ASN
1	B	48	GLN
1	B	122	GLN
1	B	404	GLN
1	C	347	HIS
1	D	49	GLN
1	D	129	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 4 are monoatomic - leaving 39 for Mogul analysis.

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	NAD	A	501	-	46,48,48	0.47	0	64,73,73	0.54	0
5	PO4	C	509	-	4,4,4	1.07	0	6,6,6	0.83	0
5	PO4	D	507	-	4,4,4	0.79	0	6,6,6	1.22	0
6	RB7	A	511	-	16,16,16	1.37	3 (18%)	22,22,22	2.37	6 (27%)
3	ADE	A	502	-	11,11,11	0.63	0	15,15,15	0.40	0
6	RB7	A	510	-	16,16,16	1.15	1 (6%)	22,22,22	2.72	8 (36%)
7	DMS	C	503	-	3,3,3	0.85	0	3,3,3	0.87	0
5	PO4	C	508	-	4,4,4	0.78	0	6,6,6	0.52	0
6	RB7	C	511	-	16,16,16	1.40	2 (12%)	22,22,22	2.60	4 (18%)
6	RB7	D	511	-	16,16,16	1.46	3 (18%)	22,22,22	2.76	6 (27%)
3	ADE	D	502	-	11,11,11	0.57	0	15,15,15	0.50	0
6	RB7	A	512	-	16,16,16	1.26	2 (12%)	22,22,22	2.90	6 (27%)
7	DMS	D	503	-	3,3,3	0.75	0	3,3,3	1.12	0
5	PO4	A	507	-	4,4,4	0.67	0	6,6,6	0.94	0
5	PO4	A	504	-	4,4,4	0.80	0	6,6,6	0.48	0
2	NAD	D	501	-	46,48,48	0.41	0	64,73,73	0.61	0
6	RB7	D	509	-	16,16,16	1.30	2 (12%)	22,22,22	2.96	6 (27%)
5	PO4	B	504	-	4,4,4	1.03	0	6,6,6	0.37	0
5	PO4	A	506	-	4,4,4	0.87	0	6,6,6	0.57	0
5	PO4	C	506	-	4,4,4	0.89	0	6,6,6	0.68	0
5	PO4	A	505	-	4,4,4	1.06	0	6,6,6	0.70	0
3	ADE	C	502	-	11,11,11	0.83	0	15,15,15	0.56	0
6	RB7	C	513	-	16,16,16	1.22	3 (18%)	22,22,22	2.49	7 (31%)
6	RB7	C	510	-	16,16,16	1.36	2 (12%)	22,22,22	2.63	7 (31%)
2	NAD	C	501	-	46,48,48	0.45	0	64,73,73	0.59	0
3	ADE	B	502	-	11,11,11	0.56	0	15,15,15	0.46	0
5	PO4	C	505	-	4,4,4	1.15	0	6,6,6	0.36	0
5	PO4	B	505	-	4,4,4	0.72	0	6,6,6	0.96	0
2	NAD	B	501	-	46,48,48	0.39	0	64,73,73	0.58	0
6	RB7	D	510	-	16,16,16	1.35	3 (18%)	22,22,22	2.51	8 (36%)
5	PO4	D	505	-	4,4,4	0.95	0	6,6,6	0.83	0
6	RB7	B	507	-	16,16,16	1.37	3 (18%)	22,22,22	2.45	5 (22%)
6	RB7	C	512	-	16,16,16	1.41	3 (18%)	22,22,22	2.63	7 (31%)
5	PO4	C	507	-	4,4,4	0.99	0	6,6,6	0.54	0
5	PO4	D	508	-	4,4,4	0.76	0	6,6,6	0.73	0
6	RB7	A	509	-	16,16,16	1.27	1 (6%)	22,22,22	3.11	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	D	506	-	4,4,4	0.72	0	6,6,6	0.62	0
6	RB7	A	508	-	16,16,16	1.35	3 (18%)	22,22,22	2.78	10 (45%)
6	RB7	B	506	-	16,16,16	1.15	1 (6%)	22,22,22	2.86	7 (31%)

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	NAD	A	501	-	-	4/30/62/62	0/5/5/5
6	RB7	A	511	-	-	3/8/8/8	0/1/1/1
6	RB7	A	510	-	-	2/8/8/8	0/1/1/1
3	ADE	A	502	-	-	-	0/2/2/2
6	RB7	C	511	-	-	4/8/8/8	0/1/1/1
6	RB7	D	511	-	-	2/8/8/8	0/1/1/1
3	ADE	D	502	-	-	-	0/2/2/2
6	RB7	A	512	-	-	4/8/8/8	0/1/1/1
2	NAD	D	501	-	-	5/30/62/62	0/5/5/5
6	RB7	D	509	-	-	3/8/8/8	0/1/1/1
3	ADE	C	502	-	-	-	0/2/2/2
6	RB7	C	513	-	-	2/8/8/8	0/1/1/1
6	RB7	C	510	-	-	5/8/8/8	0/1/1/1
2	NAD	C	501	-	-	4/30/62/62	0/5/5/5
3	ADE	B	502	-	-	-	0/2/2/2
2	NAD	B	501	-	-	4/30/62/62	0/5/5/5
6	RB7	D	510	-	-	5/8/8/8	0/1/1/1
6	RB7	B	507	-	-	2/8/8/8	0/1/1/1
6	RB7	C	512	-	-	1/8/8/8	0/1/1/1
6	RB7	A	509	-	-	2/8/8/8	0/1/1/1
6	RB7	A	508	-	-	1/8/8/8	0/1/1/1
6	RB7	B	506	-	-	0/8/8/8	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	511	RB7	C9-S	4.00	1.83	1.78
6	D	511	RB7	C9-S	3.70	1.83	1.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	509	RB7	C9-S	3.61	1.83	1.78
6	C	512	RB7	C9-S	3.60	1.83	1.78
6	C	510	RB7	C9-S	3.54	1.82	1.78
6	A	508	RB7	C9-S	3.35	1.82	1.78
6	D	509	RB7	C9-S	3.25	1.82	1.78
6	A	511	RB7	C9-S	3.20	1.82	1.78
6	D	510	RB7	BR-C6	3.14	1.96	1.89
6	B	507	RB7	C9-S	3.12	1.82	1.78
6	A	512	RB7	BR-C6	2.78	1.96	1.89
6	C	513	RB7	C9-S	2.67	1.81	1.78
6	A	512	RB7	C9-S	2.61	1.81	1.78
6	D	511	RB7	BR-C6	2.60	1.95	1.89
6	D	510	RB7	C9-S	2.54	1.81	1.78
6	A	511	RB7	BR-C6	2.40	1.95	1.89
6	B	507	RB7	BR-C6	2.40	1.95	1.89
6	D	510	RB7	C10-S	2.30	1.83	1.75
6	B	507	RB7	C10-S	2.26	1.82	1.75
6	A	511	RB7	C10-S	2.22	1.82	1.75
6	A	508	RB7	C10-S	2.19	1.82	1.75
6	C	513	RB7	O-S	2.18	1.48	1.44
6	A	510	RB7	C9-S	2.16	1.81	1.78
6	C	512	RB7	C10-S	2.14	1.82	1.75
6	D	509	RB7	C10-S	2.13	1.82	1.75
6	C	511	RB7	C10-S	2.13	1.82	1.75
6	B	506	RB7	C10-S	2.12	1.82	1.75
6	D	511	RB7	C10-S	2.11	1.82	1.75
6	A	508	RB7	C-C1	2.10	1.54	1.51
6	C	510	RB7	C10-S	2.09	1.82	1.75
6	C	512	RB7	C2-C1	-2.07	1.36	1.39
6	C	513	RB7	C10-S	2.03	1.82	1.75

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	509	RB7	O-S-O1	-9.90	98.64	117.22
6	A	509	RB7	O-S-O1	-9.76	98.92	117.22
6	D	511	RB7	O-S-O1	-9.47	99.46	117.22
6	B	506	RB7	O-S-O1	-9.22	99.92	117.22
6	C	512	RB7	O-S-O1	-8.90	100.53	117.22
6	A	509	RB7	O-S-C9	8.83	114.69	108.33
6	C	511	RB7	O-S-O1	-8.72	100.86	117.22
6	C	510	RB7	O-S-O1	-8.44	101.39	117.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	512	RB7	O-S-O1	-8.30	101.64	117.22
6	B	507	RB7	O-S-O1	-8.28	101.69	117.22
6	A	508	RB7	O-S-O1	-8.21	101.83	117.22
6	A	511	RB7	O-S-O1	-8.18	101.87	117.22
6	A	510	RB7	O-S-O1	-7.74	102.69	117.22
6	D	510	RB7	O-S-O1	-7.65	102.88	117.22
6	C	513	RB7	O-S-O1	-7.19	103.74	117.22
6	C	511	RB7	O1-S-C9	5.99	112.65	108.33
6	C	513	RB7	O-S-C9	5.90	112.58	108.33
6	A	512	RB7	O1-S-C9	5.78	112.50	108.33
6	C	512	RB7	O-S-C9	5.53	112.32	108.33
6	A	510	RB7	O1-S-C9	5.48	112.28	108.33
6	A	512	RB7	O1-S-C10	5.39	113.88	108.87
6	A	512	RB7	O-S-C9	5.21	112.08	108.33
6	B	506	RB7	O1-S-C10	5.04	113.56	108.87
6	D	511	RB7	O-S-C9	5.00	111.93	108.33
6	C	510	RB7	O1-S-C9	4.75	111.75	108.33
6	B	507	RB7	O-S-C9	4.34	111.46	108.33
6	D	509	RB7	O1-S-C9	4.34	111.46	108.33
6	A	508	RB7	O-S-C9	4.28	111.41	108.33
6	D	511	RB7	O1-S-C9	4.06	111.25	108.33
6	A	510	RB7	O-S-C9	4.04	111.24	108.33
6	B	506	RB7	O1-S-C9	3.91	111.14	108.33
6	D	509	RB7	O-S-C10	3.76	112.37	108.87
6	C	511	RB7	O-S-C9	3.72	111.01	108.33
6	A	511	RB7	O-S-C9	3.67	110.97	108.33
6	D	510	RB7	O1-S-C10	3.62	112.24	108.87
6	D	510	RB7	C8-C9-S	-3.60	104.76	112.45
6	C	510	RB7	O-S-C10	3.46	112.09	108.87
6	B	507	RB7	O1-S-C10	3.45	112.08	108.87
6	D	509	RB7	O-S-C9	3.43	110.80	108.33
6	D	509	RB7	O1-S-C10	3.36	112.00	108.87
6	C	513	RB7	O-S-C10	3.35	111.98	108.87
6	A	510	RB7	O1-S-C10	3.34	111.98	108.87
6	A	511	RB7	O1-S-C10	3.30	111.94	108.87
6	D	510	RB7	C1-C2-C3	-3.27	118.53	122.22
6	A	509	RB7	C1-C2-C3	-3.26	118.55	122.22
6	A	509	RB7	O1-S-C10	3.24	111.88	108.87
6	D	509	RB7	BR-C6-C5	3.23	123.97	117.82
6	A	508	RB7	C1-C2-C3	-3.18	118.64	122.22
6	B	506	RB7	O-S-C10	3.17	111.81	108.87
6	B	506	RB7	O-S-C9	3.14	110.59	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	508	RB7	O1-S-C9	3.10	110.56	108.33
6	D	511	RB7	O1-S-C10	3.07	111.73	108.87
6	C	510	RB7	O-S-C9	3.06	110.54	108.33
6	A	508	RB7	C-C1-C2	3.05	124.95	119.57
6	A	508	RB7	O-S-C10	3.04	111.69	108.87
6	A	510	RB7	O-S-C10	3.02	111.68	108.87
6	D	511	RB7	O-S-C10	2.94	111.61	108.87
6	C	513	RB7	O1-S-C10	2.92	111.58	108.87
6	A	508	RB7	O1-S-C10	2.86	111.53	108.87
6	D	510	RB7	O-S-C9	2.83	110.37	108.33
6	A	511	RB7	O1-S-C9	2.80	110.35	108.33
6	C	512	RB7	O1-S-C10	2.76	111.44	108.87
6	B	506	RB7	C1-C2-C3	-2.76	119.11	122.22
6	A	510	RB7	C1-C2-C3	-2.73	119.14	122.22
6	C	513	RB7	C1-C2-C3	-2.64	119.24	122.22
6	B	507	RB7	C2-C1-C6	2.63	120.88	116.87
6	C	510	RB7	C1-C2-C3	-2.60	119.30	122.22
6	D	510	RB7	C4-C3-C2	2.59	122.12	118.55
6	A	508	RB7	C4-C3-C2	2.59	122.11	118.55
6	A	508	RB7	C8-C9-S	-2.55	107.02	112.45
6	A	508	RB7	C7-C3-C4	-2.53	115.77	120.94
6	C	510	RB7	O1-S-C10	2.50	111.20	108.87
6	D	510	RB7	C2-C1-C6	2.50	120.68	116.87
6	B	507	RB7	C1-C2-C3	-2.42	119.50	122.22
6	C	512	RB7	C1-C2-C3	-2.38	119.54	122.22
6	C	512	RB7	O-S-C10	2.38	111.08	108.87
6	A	511	RB7	C1-C2-C3	-2.35	119.57	122.22
6	D	510	RB7	BR-C6-C5	2.30	122.21	117.82
6	A	512	RB7	C1-C2-C3	-2.29	119.63	122.22
6	C	512	RB7	O1-S-C9	2.29	109.98	108.33
6	C	511	RB7	O-S-C10	2.28	110.99	108.87
6	B	506	RB7	C4-C3-C2	2.21	121.60	118.55
6	C	513	RB7	C7-N-C8	-2.19	105.50	113.20
6	C	513	RB7	C4-C3-C2	2.18	121.56	118.55
6	C	510	RB7	C-C1-C2	2.16	123.37	119.57
6	D	511	RB7	C1-C2-C3	-2.12	119.83	122.22
6	A	512	RB7	C2-C1-C6	2.08	120.05	116.87
6	A	510	RB7	C4-C3-C2	2.07	121.40	118.55
6	A	511	RB7	C2-C1-C6	2.07	120.02	116.87
6	A	509	RB7	C2-C1-C6	2.06	120.01	116.87
6	C	512	RB7	C4-C3-C2	2.02	121.33	118.55
6	A	510	RB7	C7-C3-C2	-2.02	116.32	120.63

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	C	501	NAD	O4D-C1D-N1N-C2N
2	C	501	NAD	O4D-C1D-N1N-C6N
2	C	501	NAD	C2D-C1D-N1N-C2N
2	C	501	NAD	C2D-C1D-N1N-C6N
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C2D-C1D-N1N-C2N
2	D	501	NAD	C2D-C1D-N1N-C6N
6	A	509	RB7	N-C8-C9-S
6	A	510	RB7	C8-C9-S-O1
6	A	512	RB7	C8-C9-S-C10
6	A	512	RB7	C8-C9-S-O1
6	C	510	RB7	N-C8-C9-S
6	C	510	RB7	C8-C9-S-C10
6	C	510	RB7	C8-C9-S-O1
6	C	510	RB7	C8-C9-S-O
6	C	511	RB7	C8-C9-S-C10
6	C	511	RB7	C8-C9-S-O1
6	C	511	RB7	C8-C9-S-O
6	C	513	RB7	C8-C9-S-O1
6	D	509	RB7	C8-C9-S-C10
6	D	509	RB7	C8-C9-S-O1
6	D	510	RB7	N-C8-C9-S
6	D	510	RB7	C8-C9-S-C10
6	D	510	RB7	C8-C9-S-O1
6	D	510	RB7	C8-C9-S-O
6	A	509	RB7	C3-C7-N-C8
6	B	507	RB7	C3-C7-N-C8
6	A	510	RB7	C9-C8-N-C7
6	C	513	RB7	C9-C8-N-C7
6	D	509	RB7	C9-C8-N-C7
6	A	512	RB7	C3-C7-N-C8

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Mol	Chain	Res	Type	Atoms
6	D	511	RB7	C3-C7-N-C8
6	A	511	RB7	C9-C8-N-C7
6	D	510	RB7	C9-C8-N-C7
6	A	508	RB7	C8-C9-S-C10
6	A	511	RB7	C8-C9-S-C10
6	A	512	RB7	C9-C8-N-C7
6	C	512	RB7	C9-C8-N-C7
6	D	511	RB7	C9-C8-N-C7
6	C	511	RB7	C3-C7-N-C8
6	B	507	RB7	C8-C9-S-C10
2	D	501	NAD	O4B-C4B-C5B-O5B
6	A	511	RB7	C8-C9-S-O
6	C	510	RB7	C9-C8-N-C7

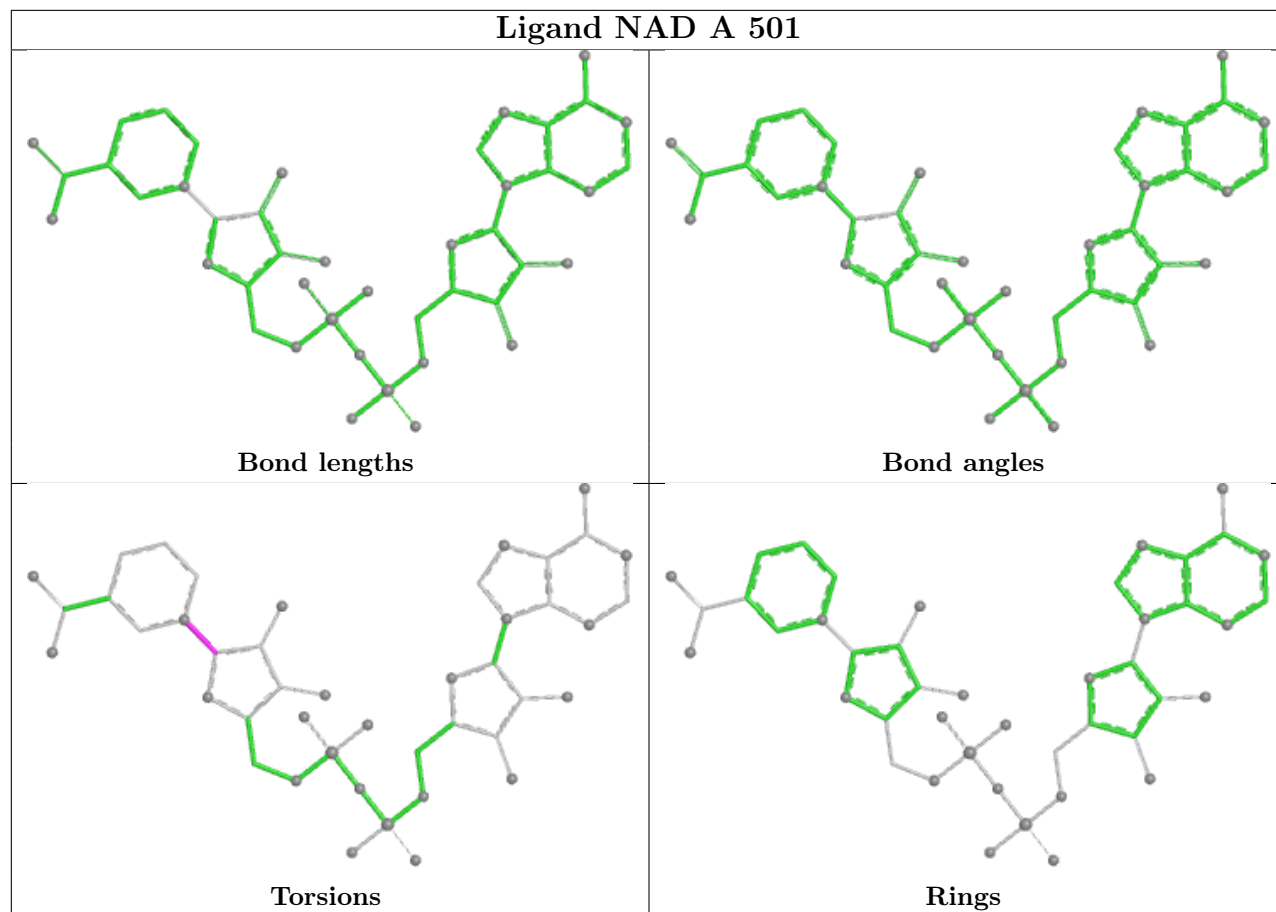
There are no ring outliers.

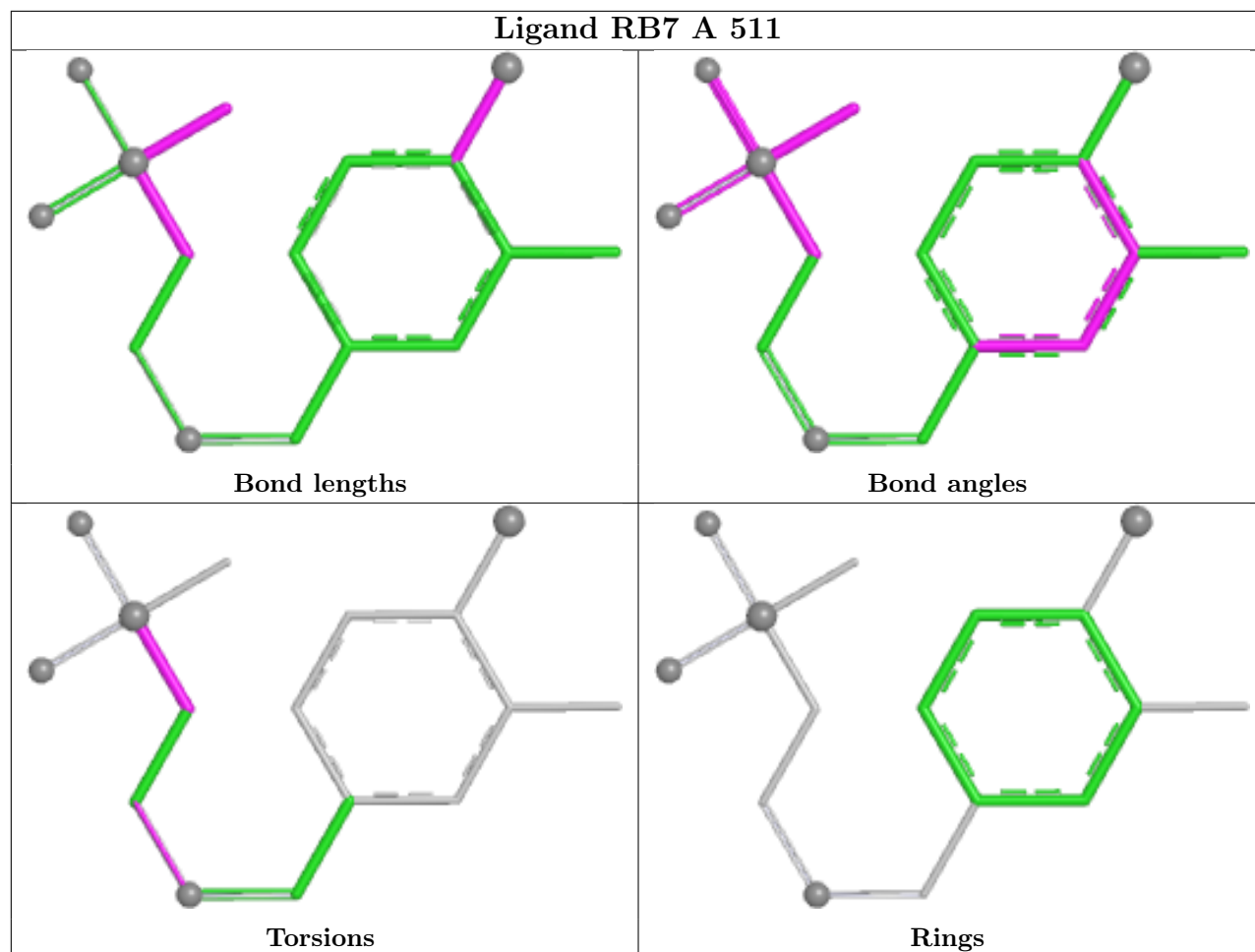
12 monomers are involved in 19 short contacts:

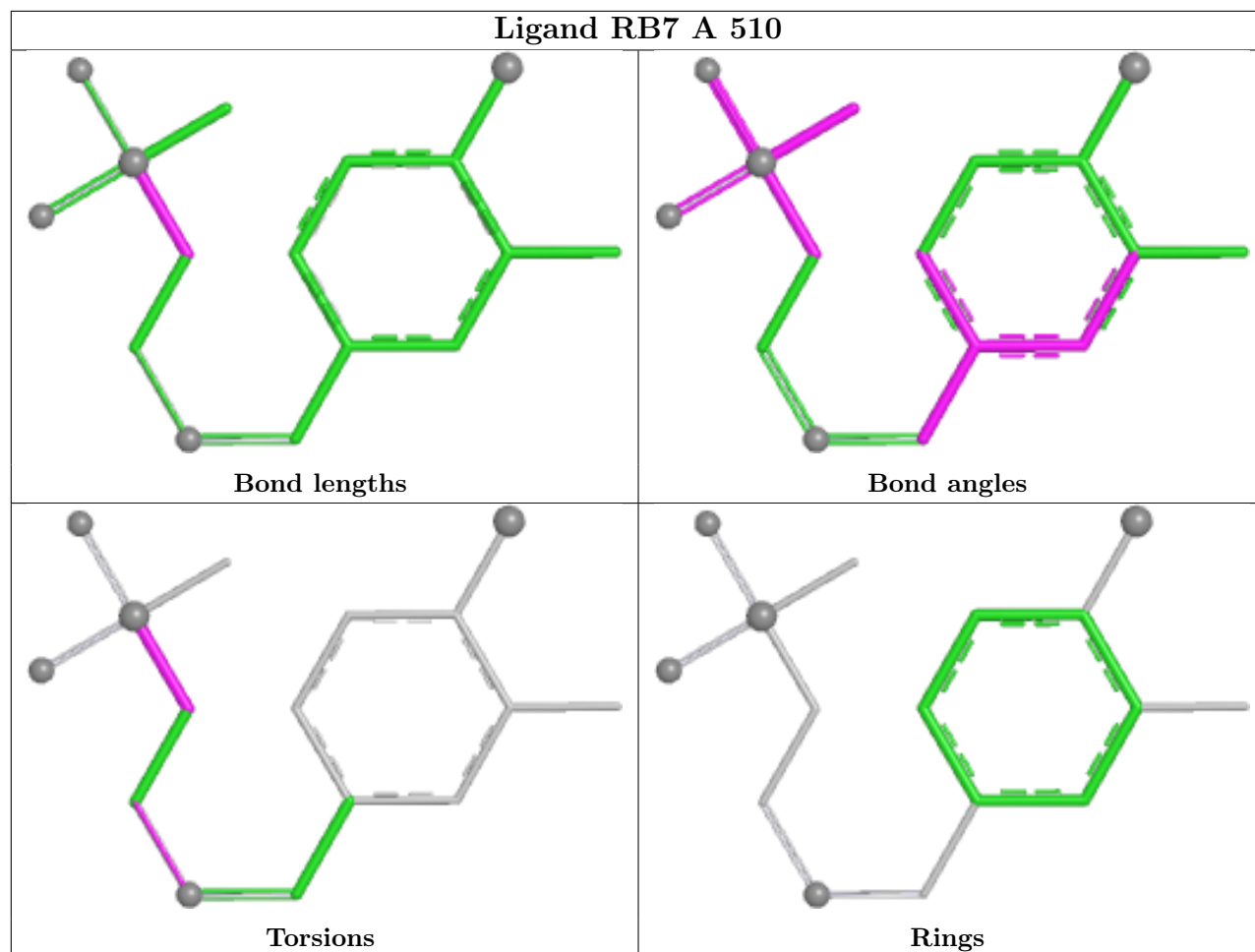
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	509	PO4	1	0
6	A	510	RB7	3	0
6	A	512	RB7	1	0
5	A	507	PO4	1	0
2	D	501	NAD	1	0
6	C	513	RB7	3	0
2	C	501	NAD	1	0
5	C	505	PO4	1	0
6	D	510	RB7	2	0
5	D	505	PO4	1	0
6	A	509	RB7	1	0
6	B	506	RB7	3	0

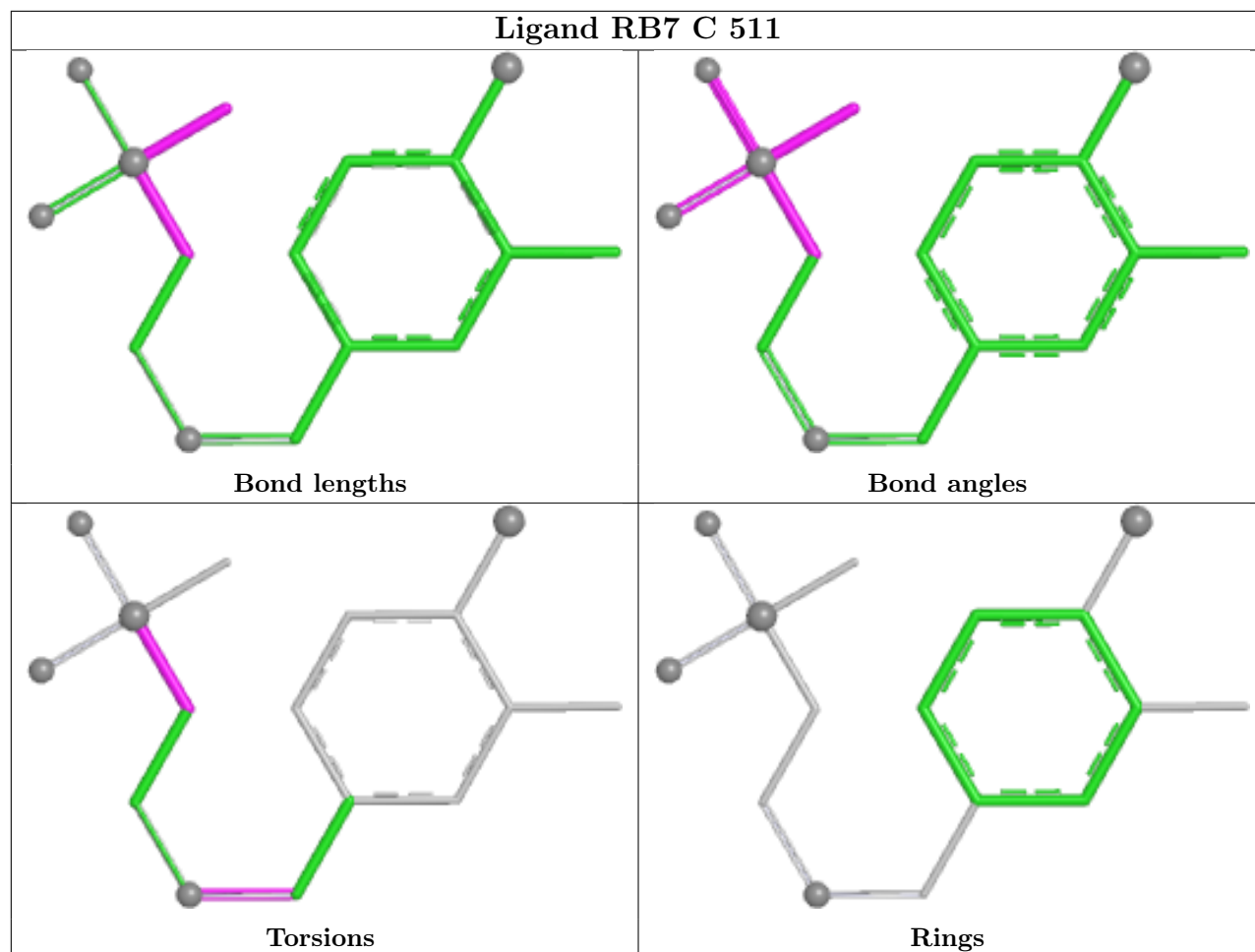
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

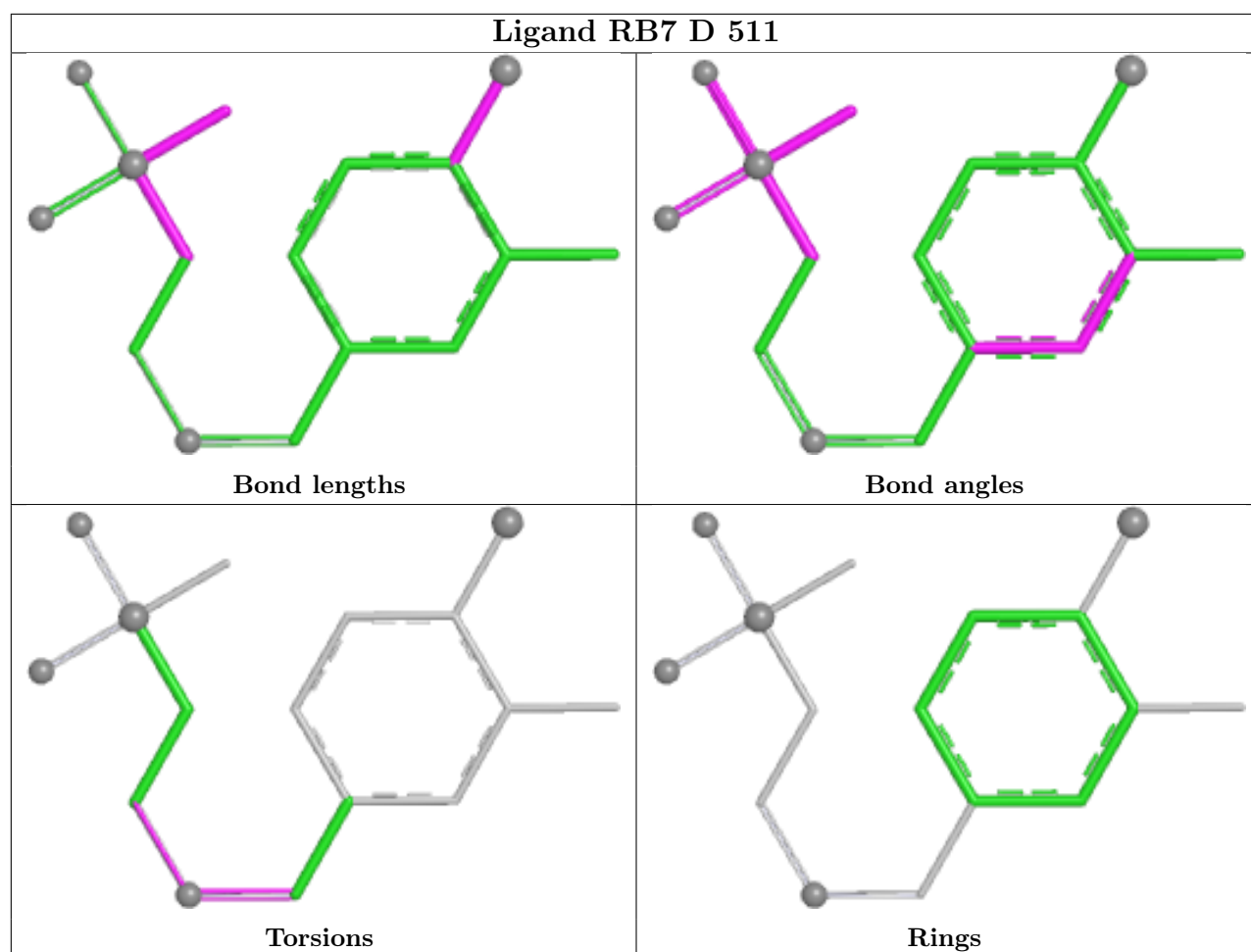
equivalents in the CSD to analyse the geometry.

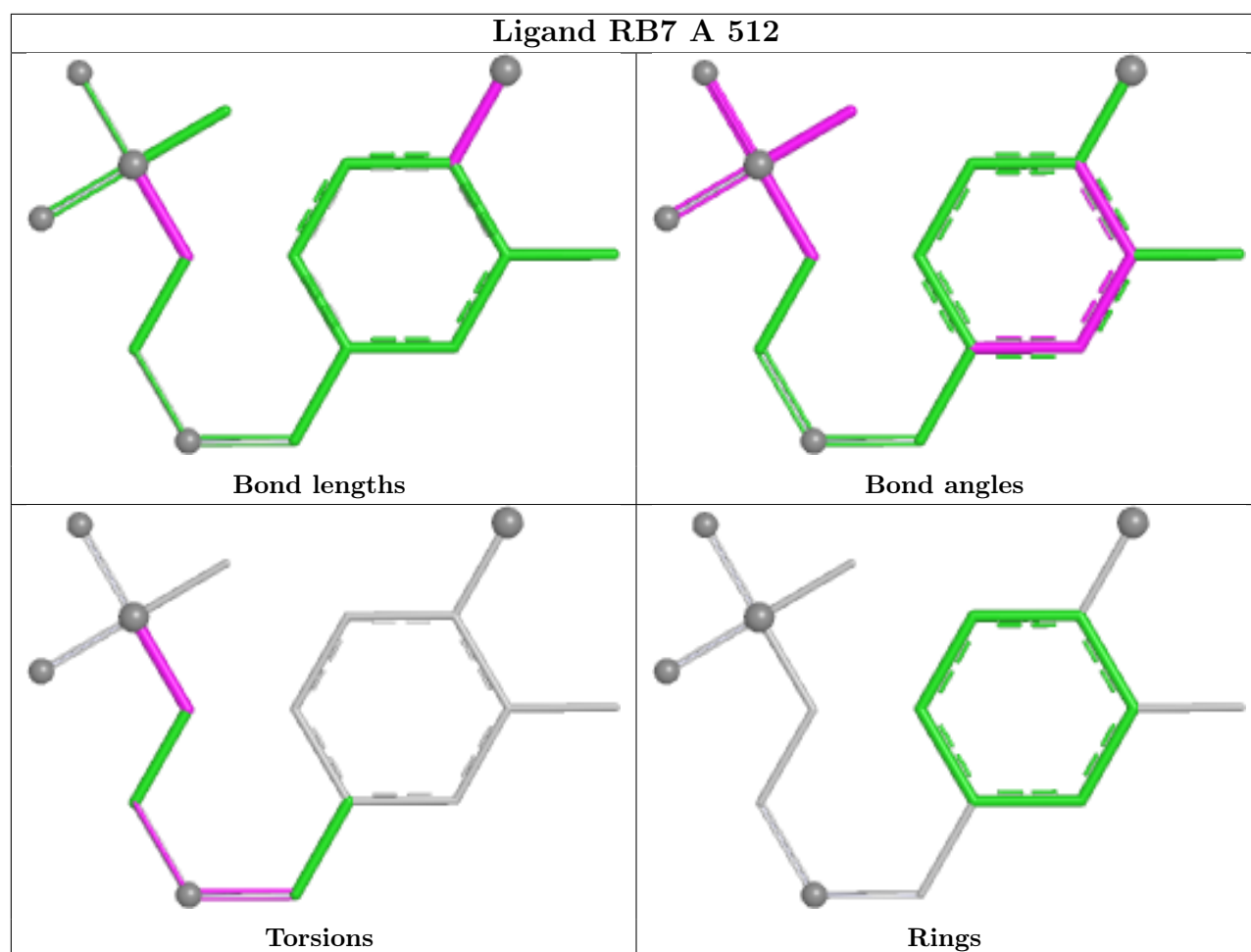


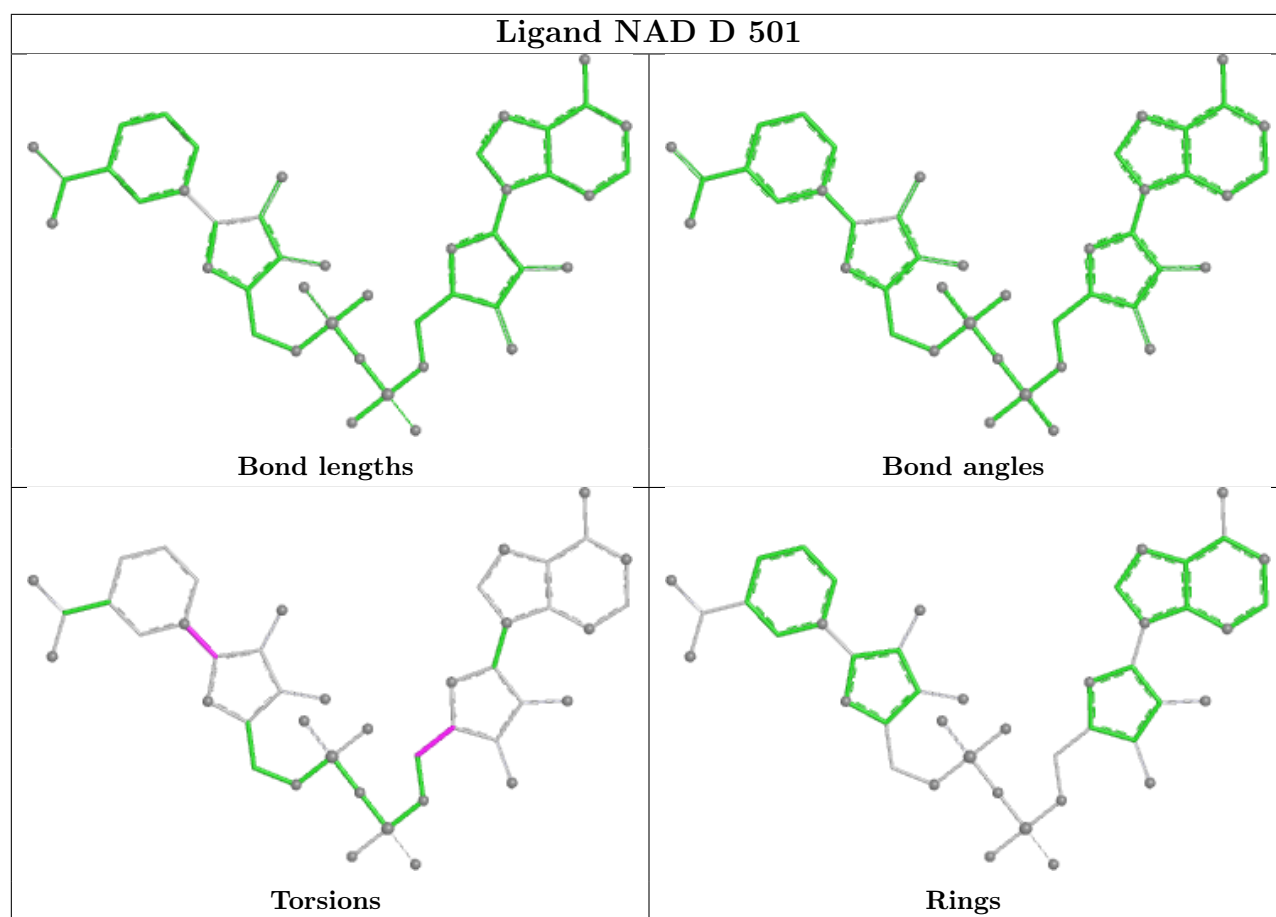


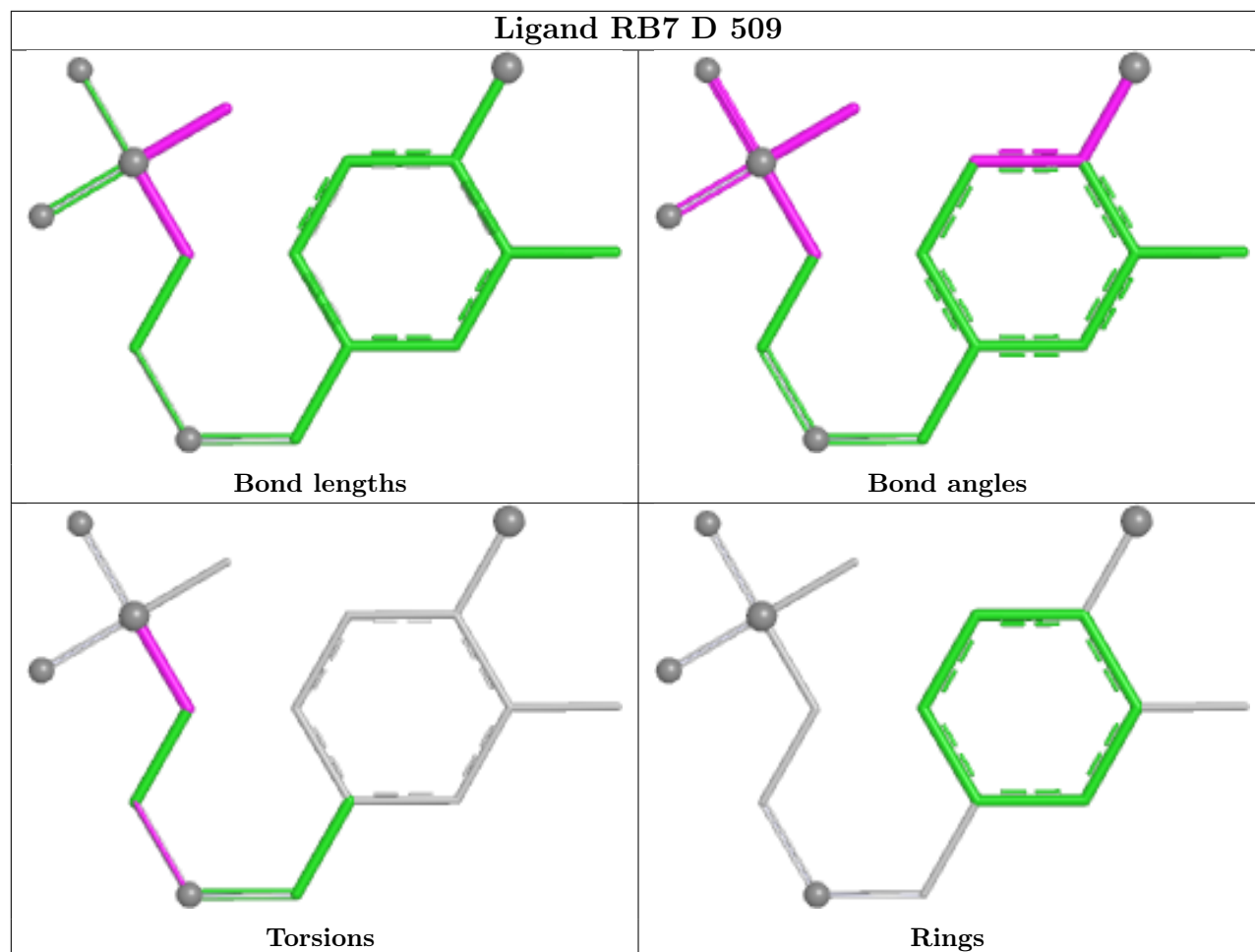


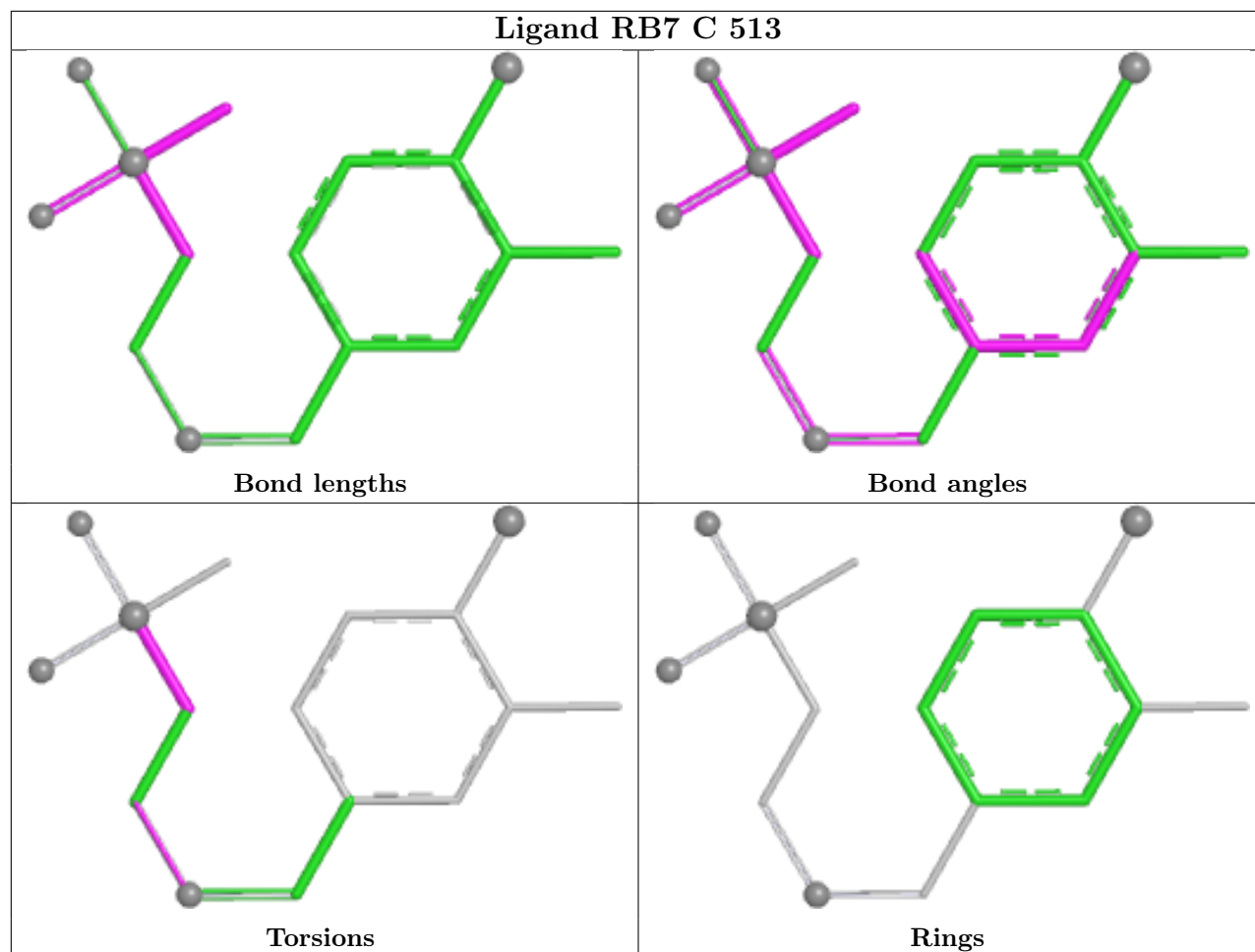


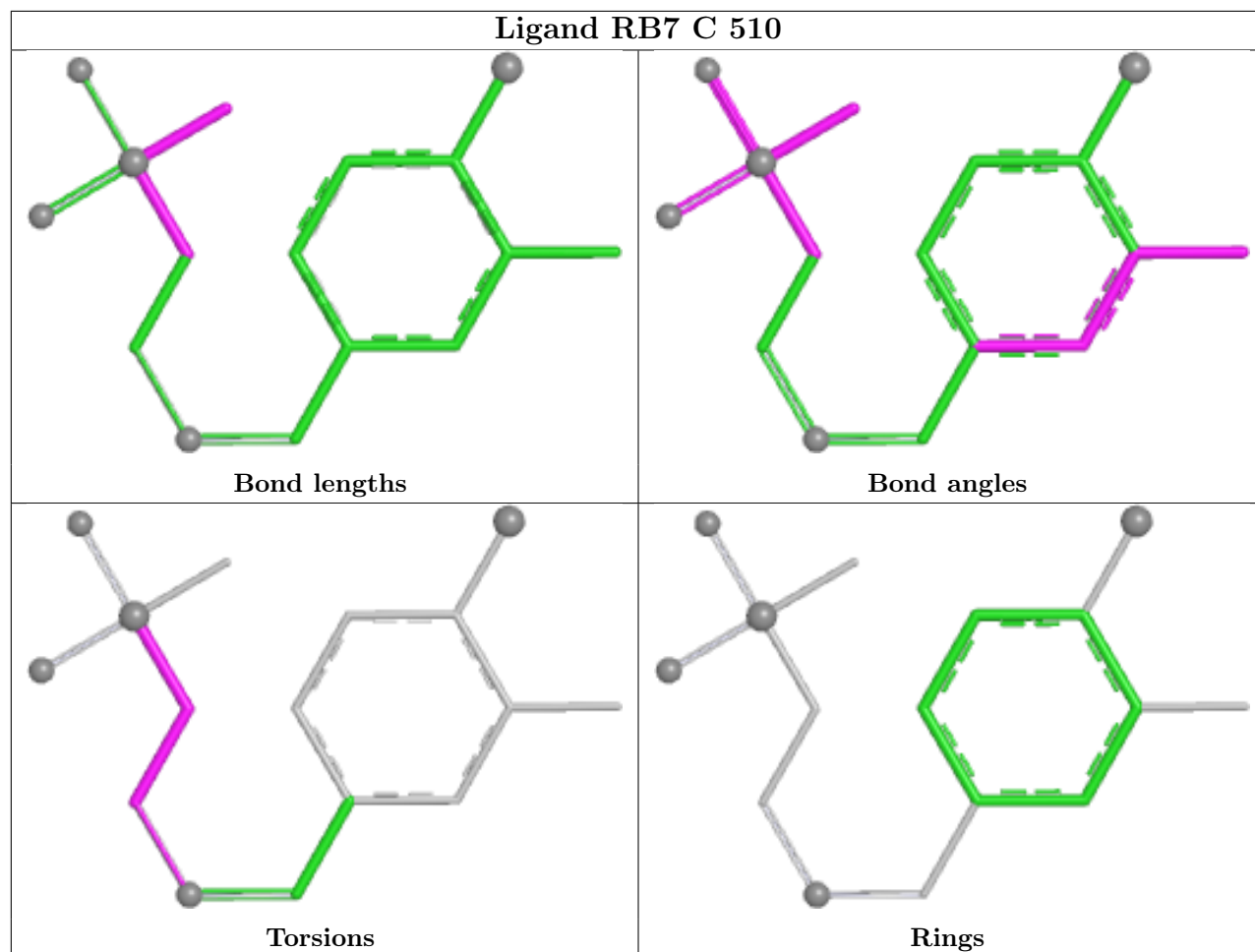


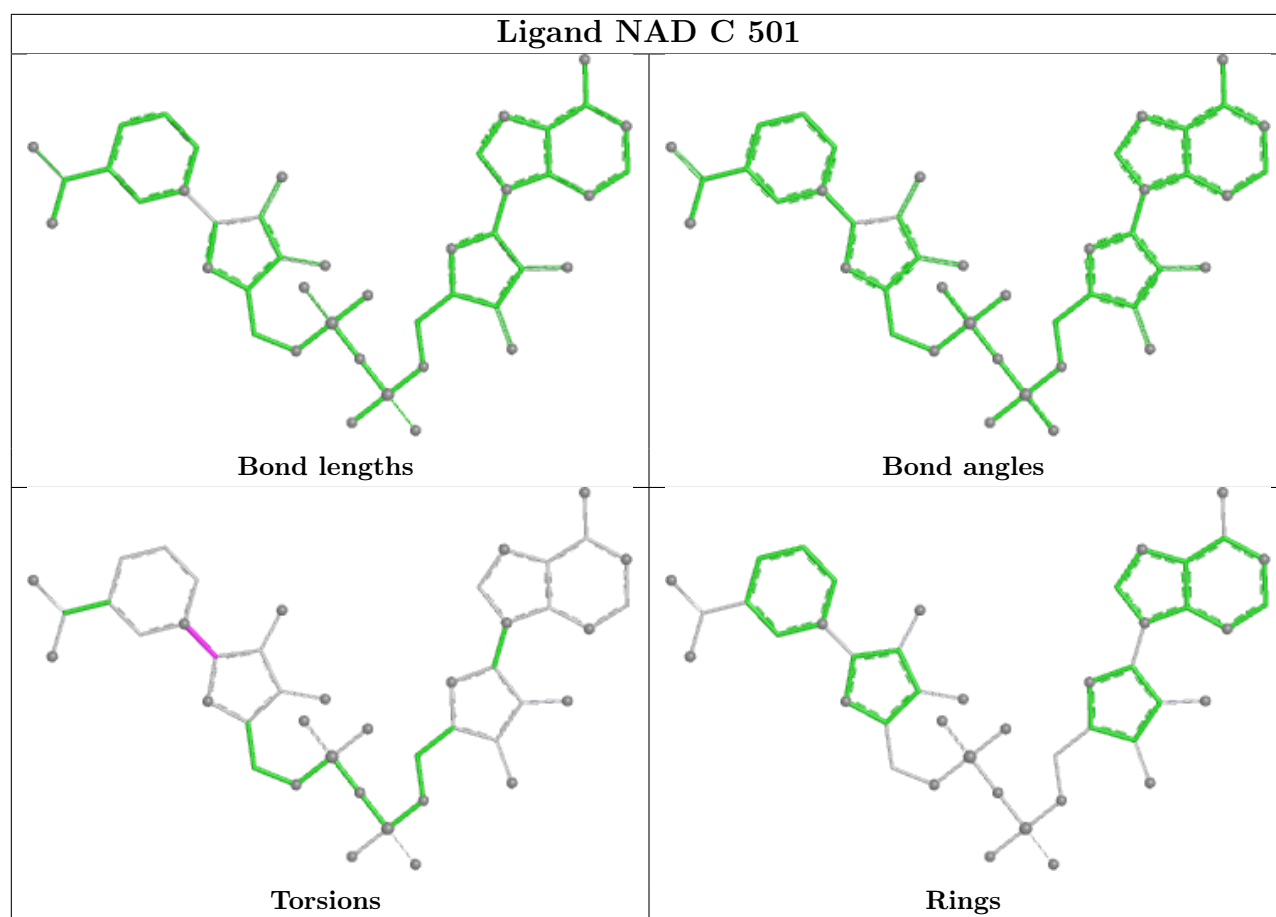


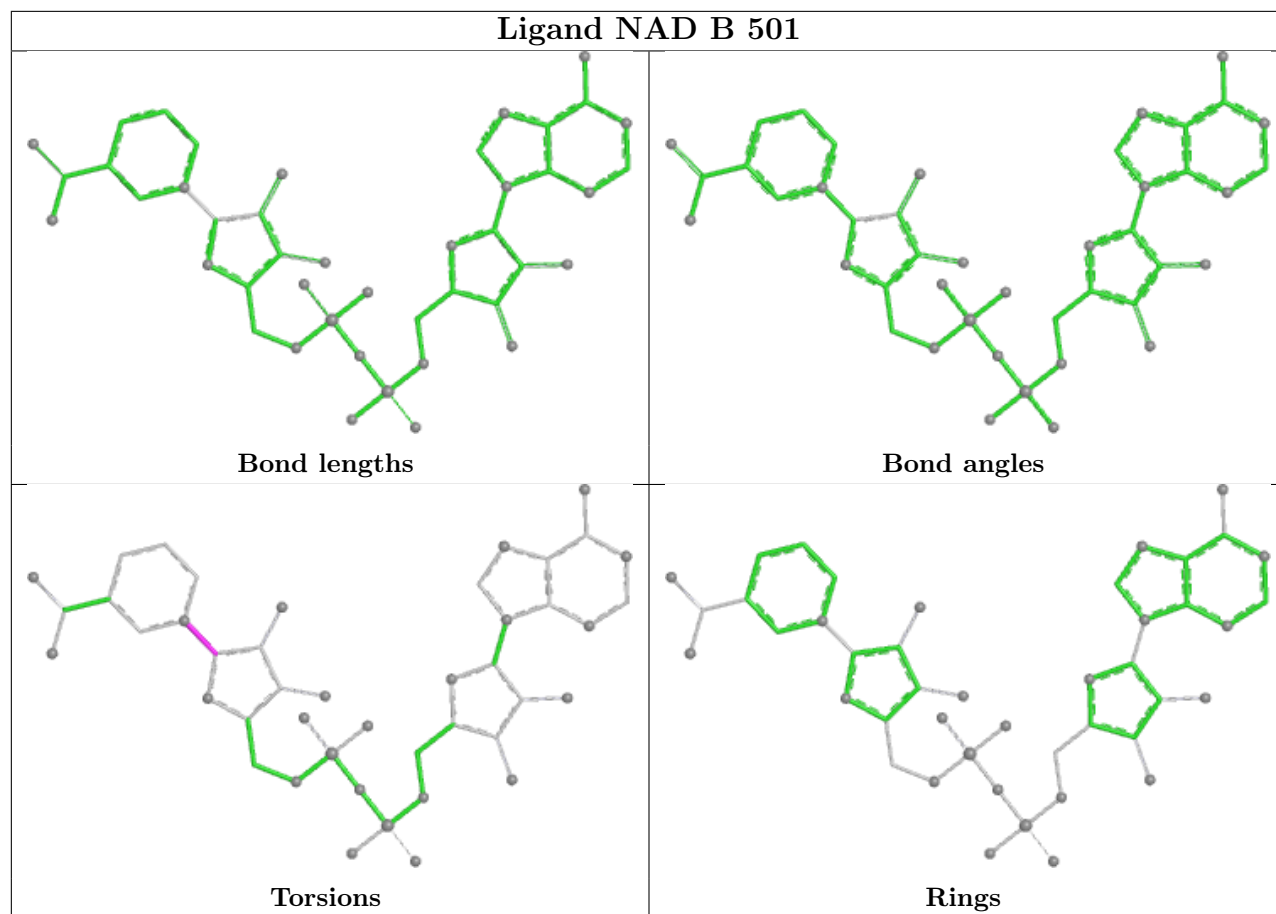


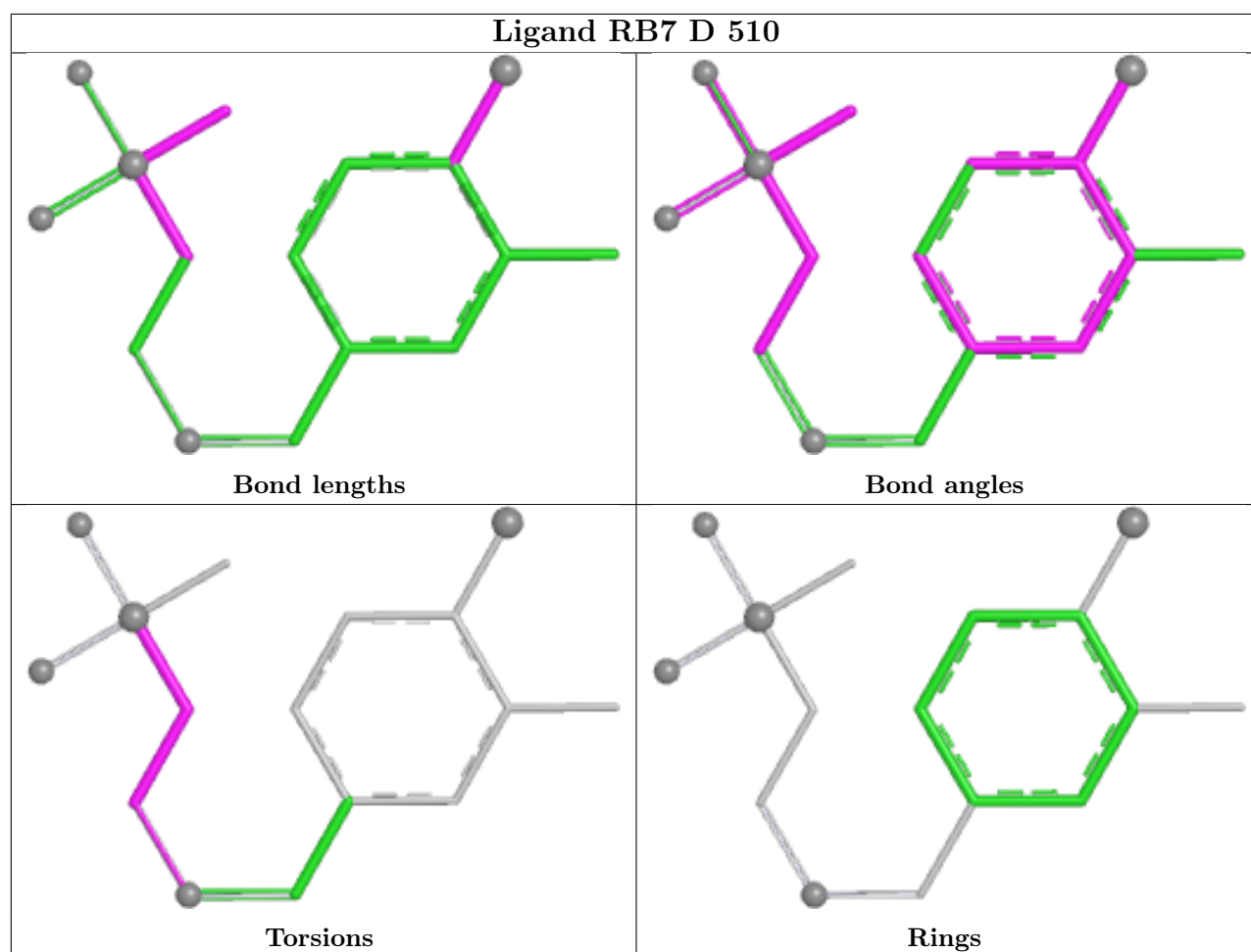


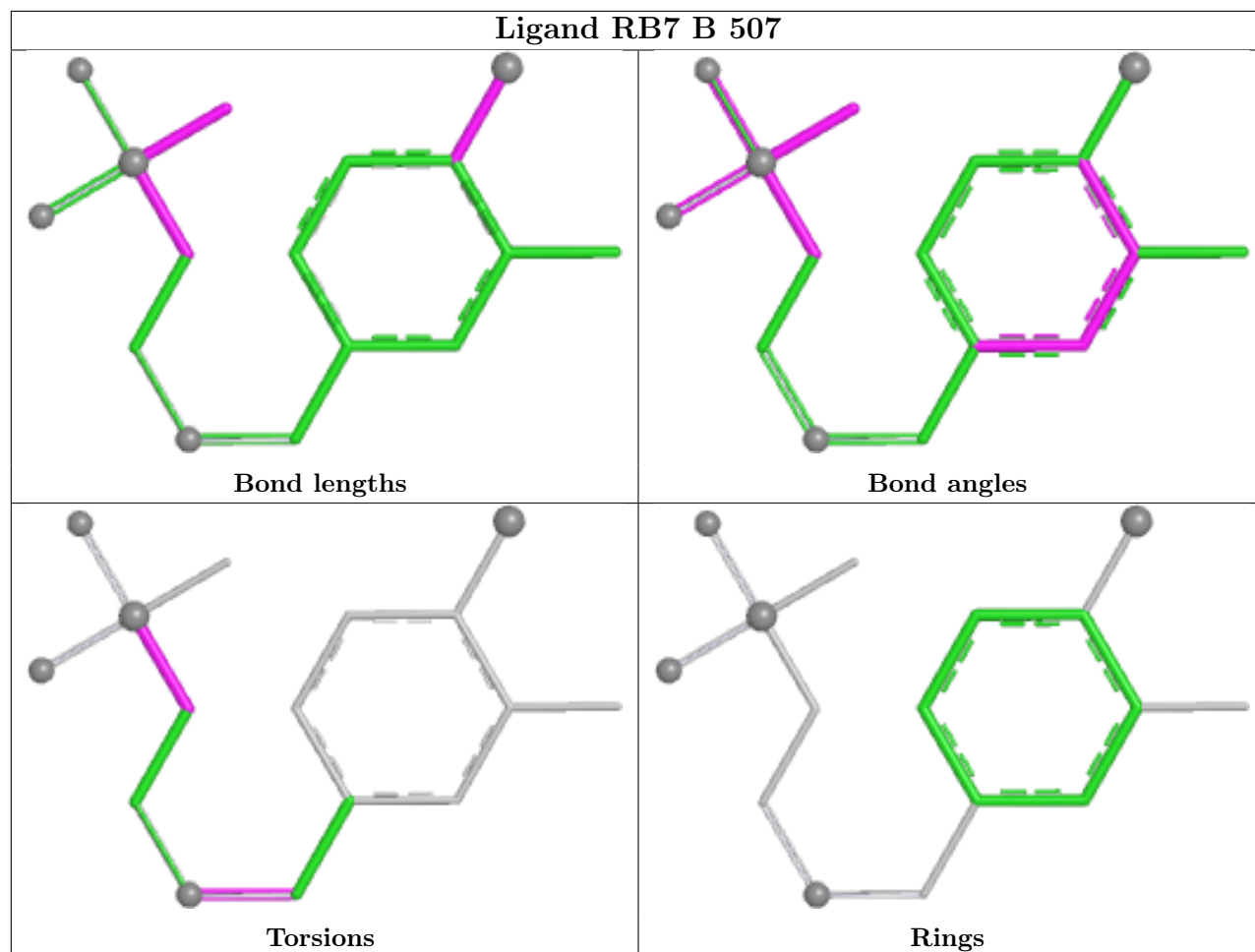


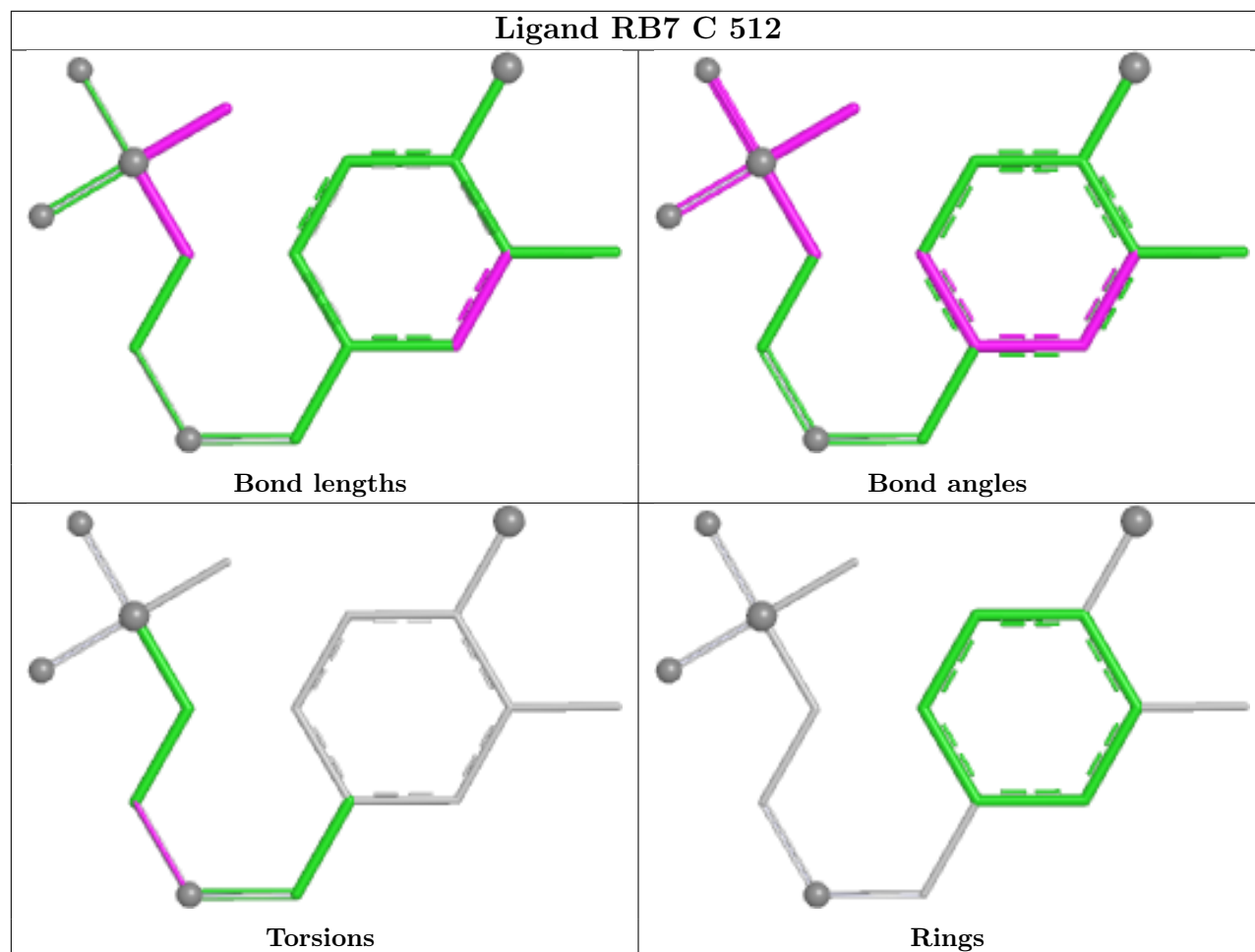


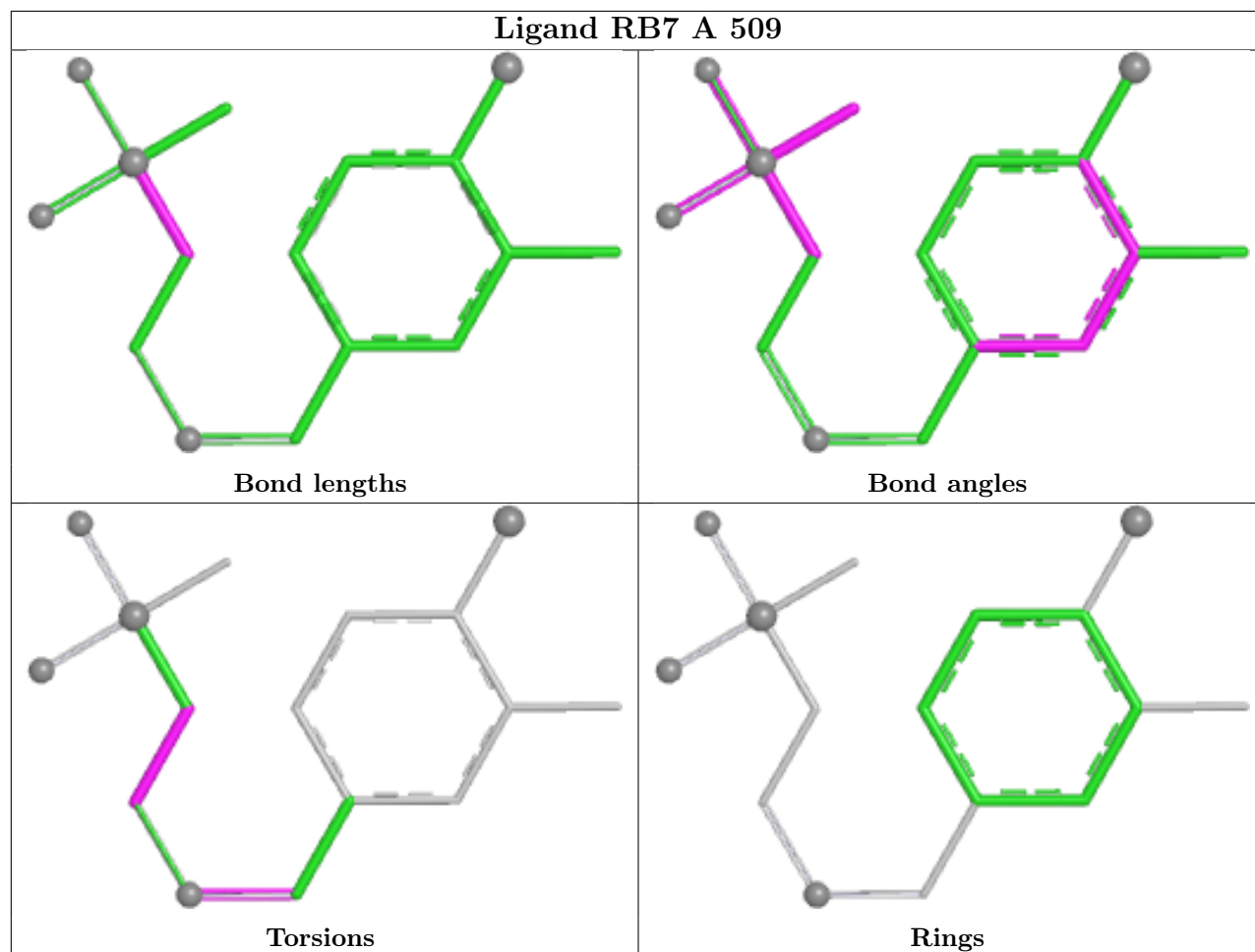


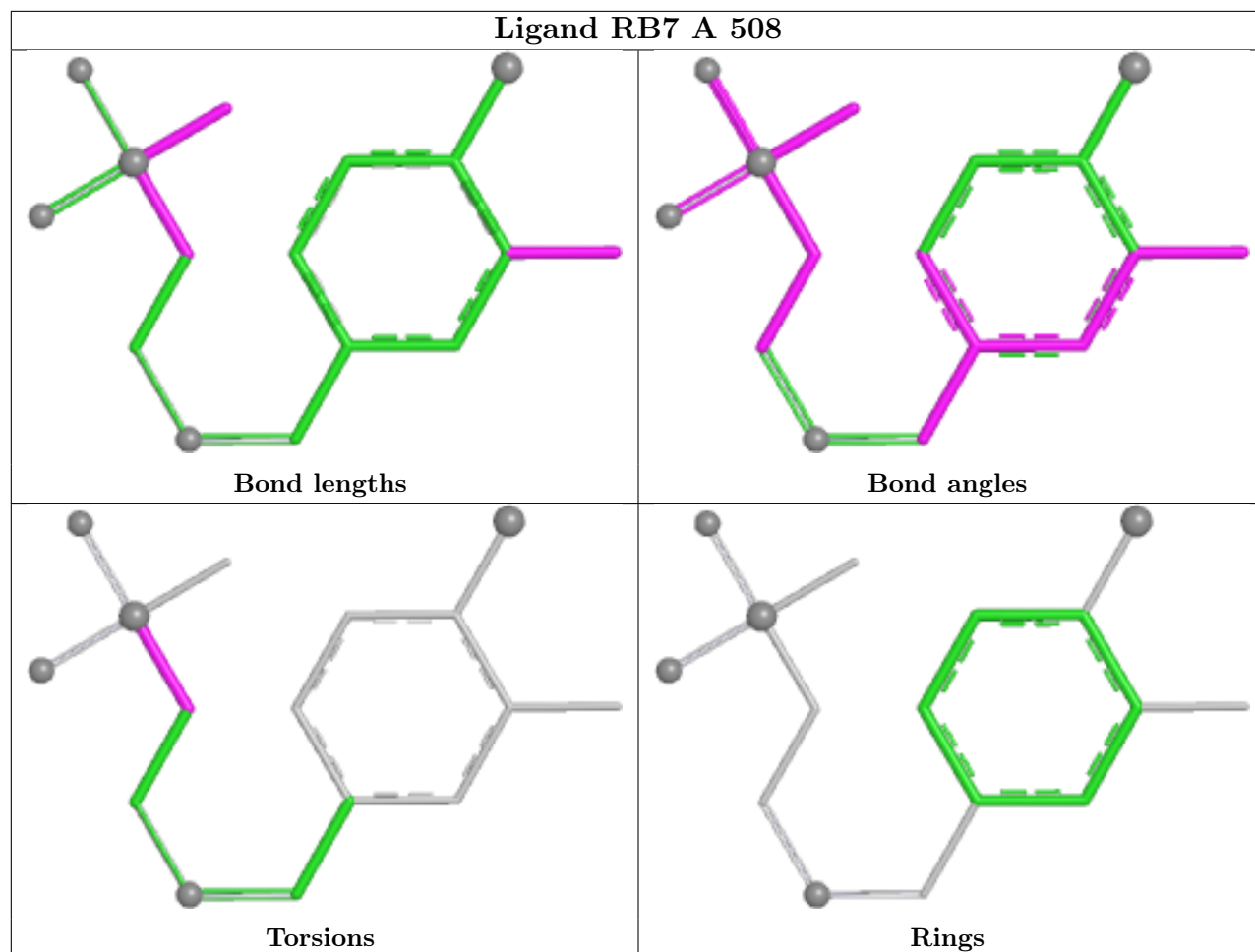


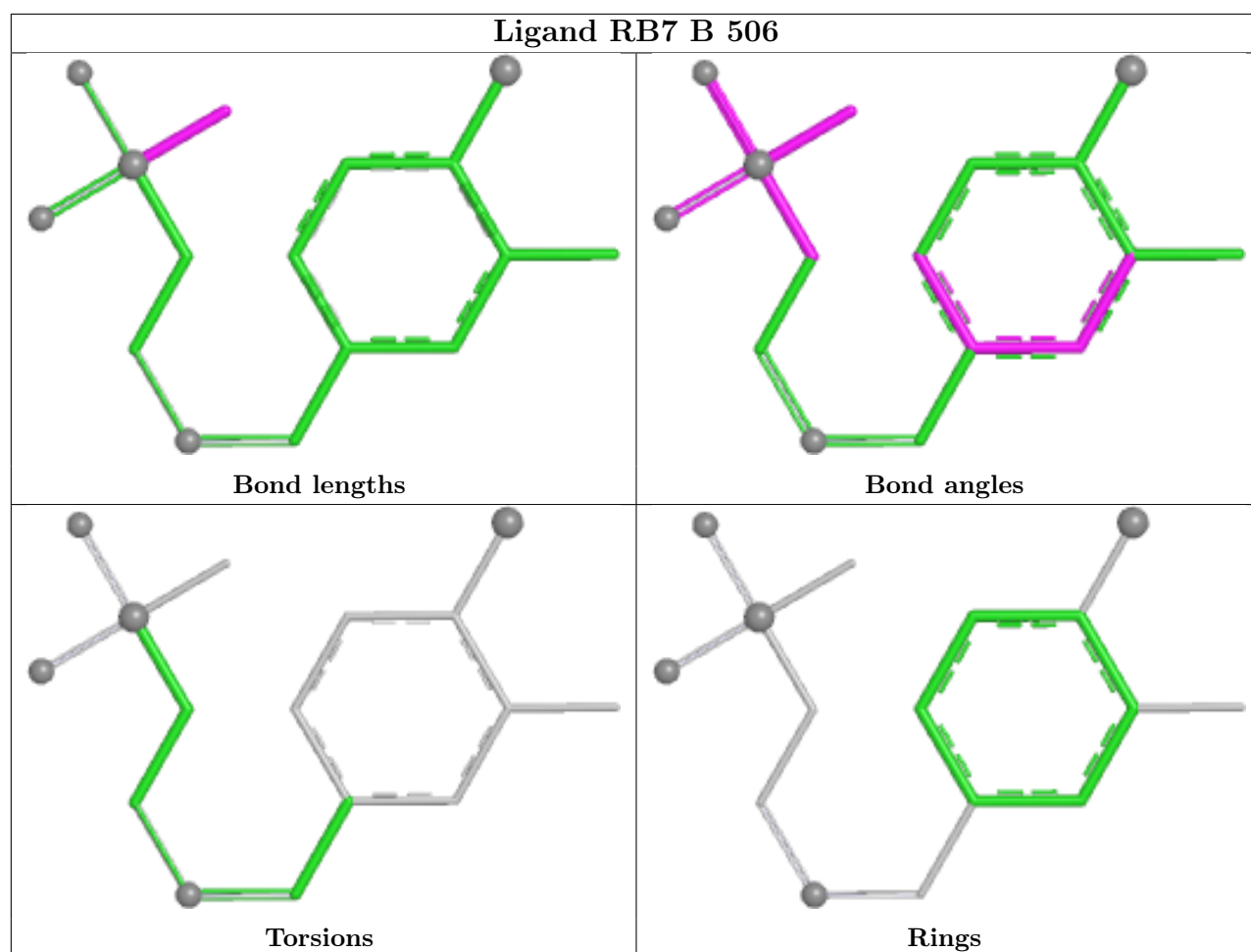












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	462/472 (97%)	-0.40	0 100 100	18, 45, 64, 109	6 (1%)
1	B	461/472 (97%)	-0.32	1 (0%) 91 93	17, 45, 72, 93	4 (0%)
1	C	462/472 (97%)	-0.39	2 (0%) 88 91	18, 44, 69, 98	10 (2%)
1	D	461/472 (97%)	-0.35	1 (0%) 91 93	18, 45, 66, 90	5 (1%)
All	All	1846/1888 (97%)	-0.36	4 (0%) 91 93	17, 45, 68, 109	25 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	GLY	4.1
1	D	39[A]	MET	3.4
1	C	8	ALA	2.3
1	B	400	HIS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

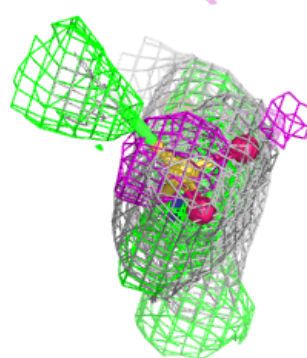
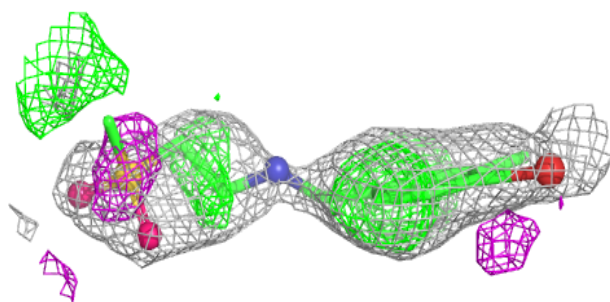
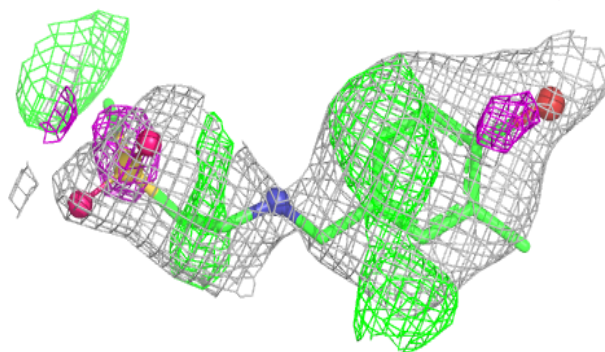
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	RB7	D	510	16/16	0.74	0.20	43,59,89,122	16
6	RB7	A	512	16/16	0.80	0.16	57,71,83,93	32
6	RB7	A	508	16/16	0.81	0.17	41,57,97,101	16
6	RB7	A	509	16/16	0.84	0.17	49,69,81,83	16
6	RB7	C	510	16/16	0.85	0.15	49,59,81,83	16
6	RB7	A	511	16/16	0.85	0.16	63,79,99,99	32
6	RB7	C	512	16/16	0.86	0.15	71,88,108,114	32
6	RB7	B	507	16/16	0.86	0.14	62,83,116,116	32
6	RB7	D	511	16/16	0.86	0.15	62,75,92,93	32
5	PO4	D	508	5/5	0.87	0.13	45,46,55,59	5
6	RB7	C	513	16/16	0.87	0.15	62,75,89,89	32
7	DMS	C	503	4/4	0.87	0.13	44,47,64,69	0
6	RB7	C	511	16/16	0.88	0.14	49,61,97,98	16
6	RB7	B	506	16/16	0.88	0.13	56,67,73,74	32
5	PO4	C	508	5/5	0.89	0.10	44,48,56,57	5
7	DMS	D	503	4/4	0.89	0.14	45,49,53,64	4
5	PO4	A	504	5/5	0.90	0.08	61,63,68,69	0
5	PO4	A	505	5/5	0.90	0.10	48,48,50,52	5
5	PO4	A	506	5/5	0.90	0.15	56,62,63,66	0
5	PO4	C	507	5/5	0.90	0.10	50,50,55,58	5
5	PO4	C	509	5/5	0.92	0.10	46,46,50,52	5
5	PO4	D	505	5/5	0.92	0.10	41,47,48,53	5
5	PO4	D	506	5/5	0.92	0.15	51,55,61,64	0
6	RB7	A	510	16/16	0.92	0.13	57,68,79,79	32
5	PO4	B	505	5/5	0.93	0.09	35,41,43,47	0
5	PO4	B	504	5/5	0.94	0.10	41,43,44,48	5
6	RB7	D	509	16/16	0.94	0.12	52,59,62,71	16
5	PO4	D	507	5/5	0.95	0.07	36,38,42,45	5
5	PO4	C	506	5/5	0.96	0.07	41,41,46,49	0
3	ADE	A	502	10/10	0.96	0.06	38,40,42,44	0
2	NAD	D	501	44/44	0.96	0.06	31,38,41,45	0
5	PO4	C	505	5/5	0.96	0.07	45,46,51,54	5
2	NAD	B	501	44/44	0.97	0.06	30,35,39,40	0
2	NAD	C	501	44/44	0.97	0.06	32,38,41,42	0
3	ADE	C	502	10/10	0.97	0.06	36,42,50,52	0
5	PO4	A	507	5/5	0.98	0.05	39,40,43,47	5
3	ADE	B	502	10/10	0.98	0.05	37,40,41,41	0
2	NAD	A	501	44/44	0.98	0.05	31,36,39,40	0
3	ADE	D	502	10/10	0.98	0.04	33,38,41,41	0
4	K	B	503	1/1	0.99	0.04	36,36,36,36	0
4	K	D	504	1/1	0.99	0.05	36,36,36,36	0
4	K	A	503	1/1	0.99	0.04	36,36,36,36	0
4	K	C	504	1/1	1.00	0.03	39,39,39,39	0

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

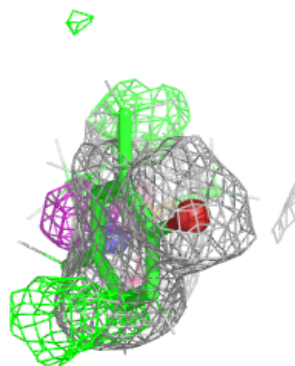
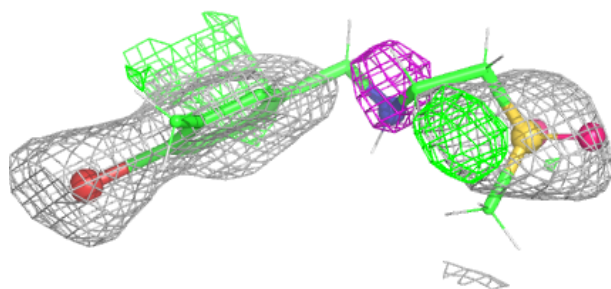
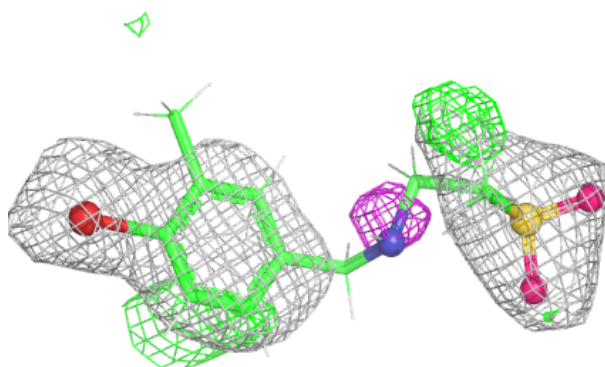
Electron density around RB7 D 510:

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

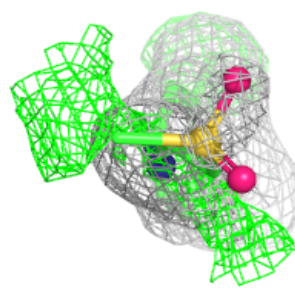
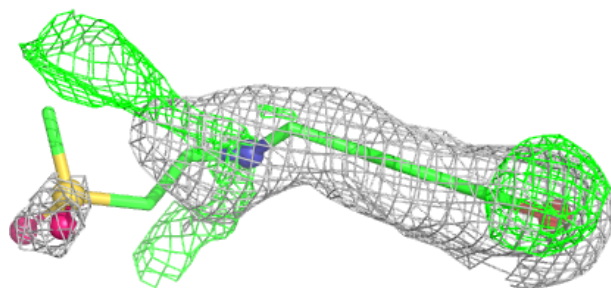
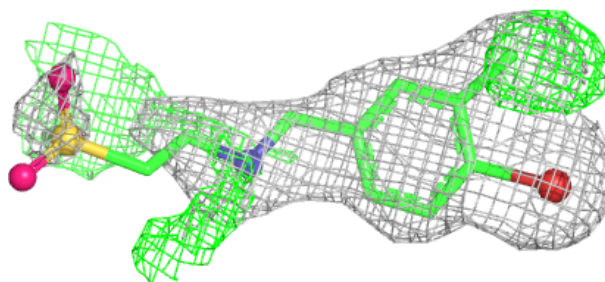


Electron density around RB7 A 512:

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

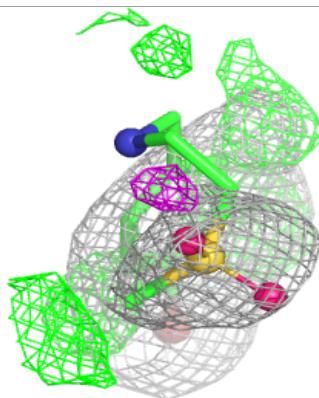
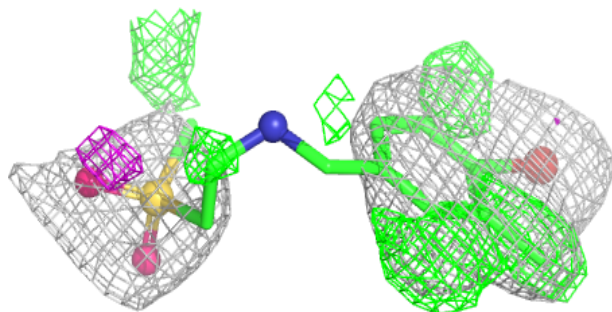
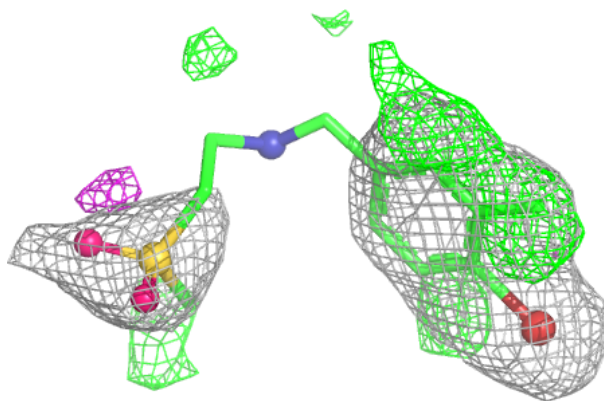
**Electron density around RB7 A 508:**

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

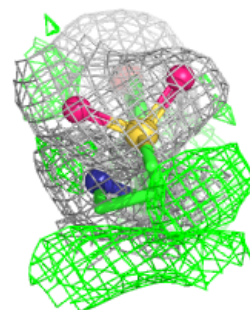
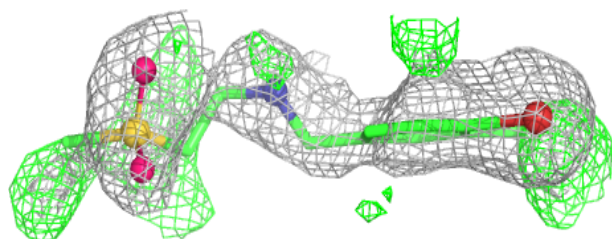
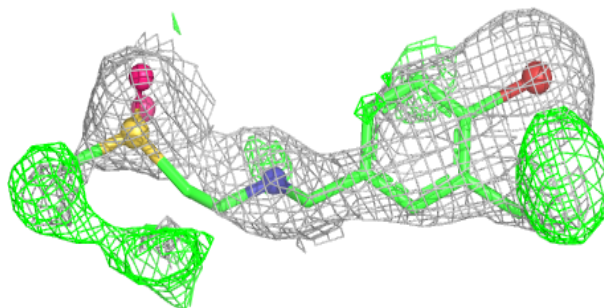


Electron density around RB7 A 509:

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

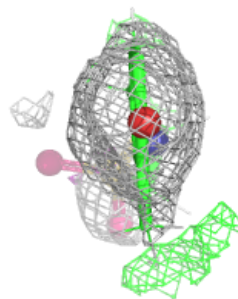
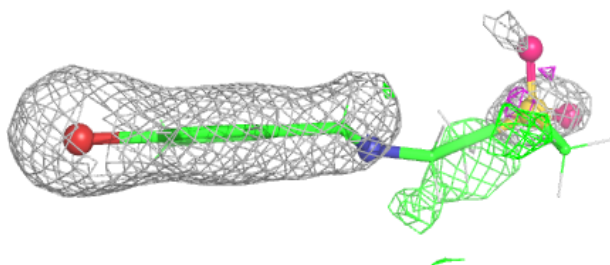
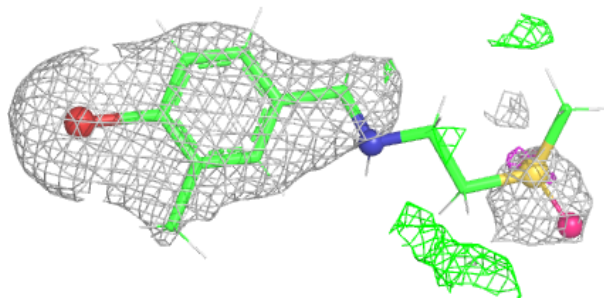
**Electron density around RB7 C 510:**

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

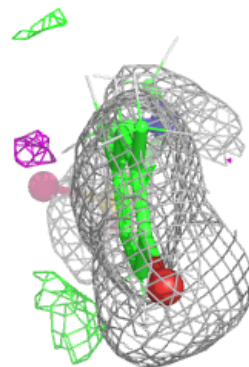
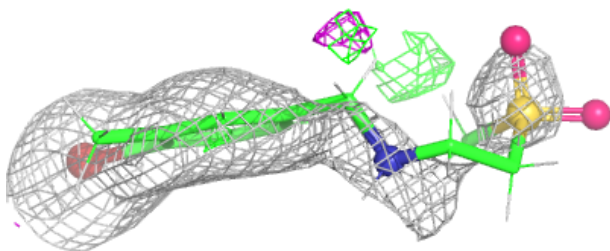
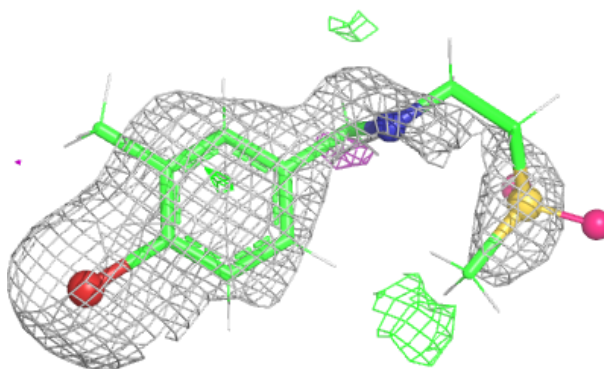


Electron density around RB7 A 511:

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

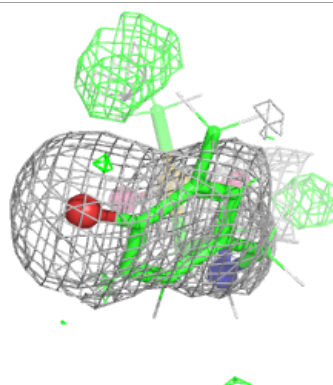
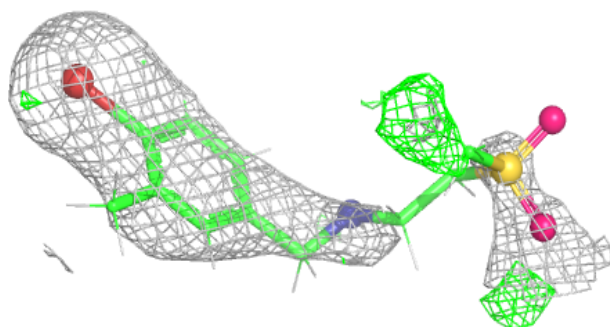
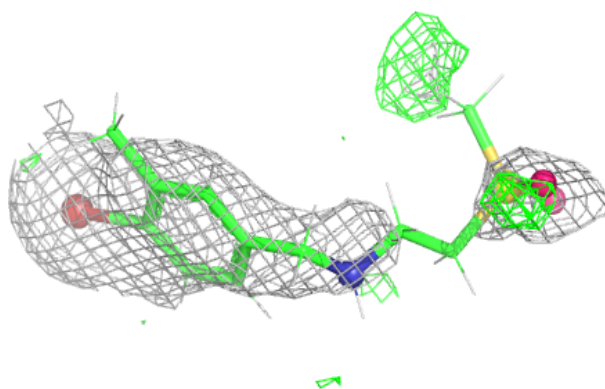
**Electron density around RB7 C 512:**

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

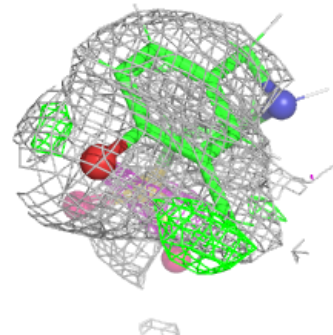
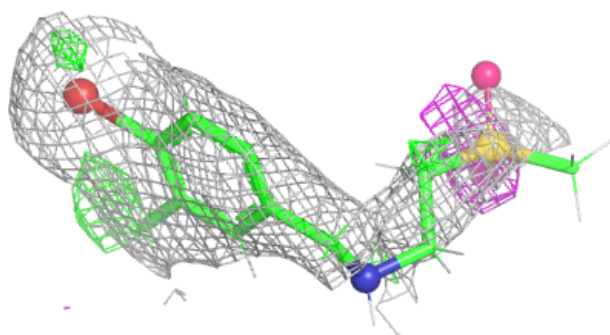
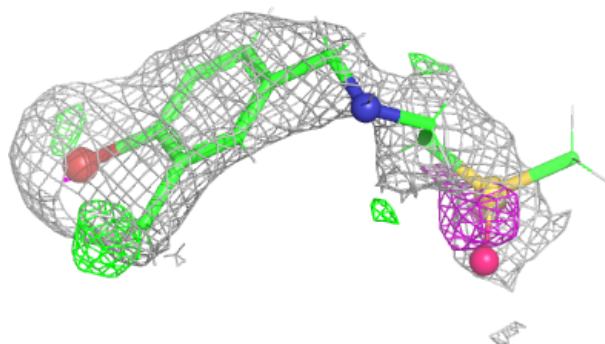


Electron density around RB7 B 507:

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

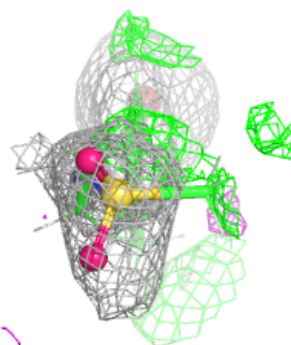
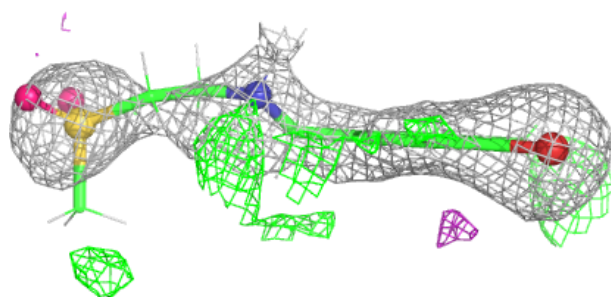
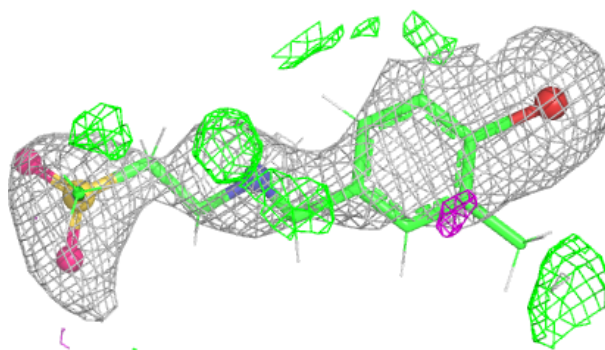
**Electron density around RB7 D 511:**

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

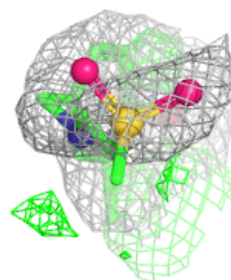
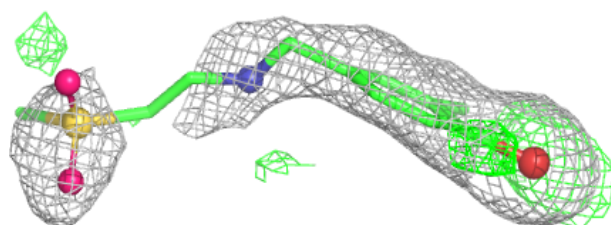
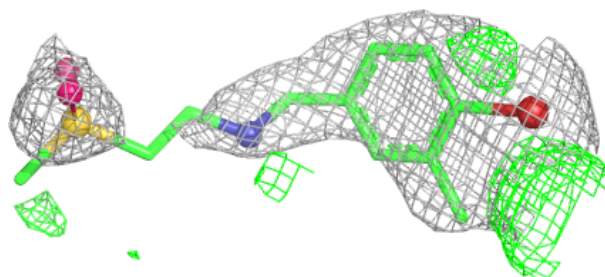


Electron density around RB7 C 513:

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

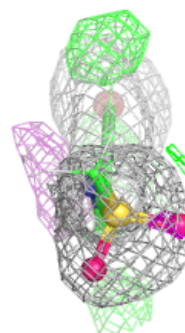
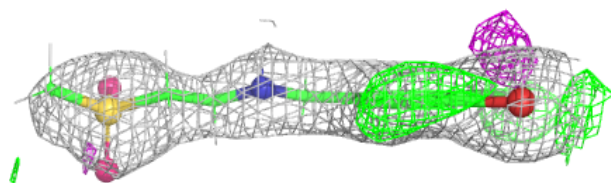
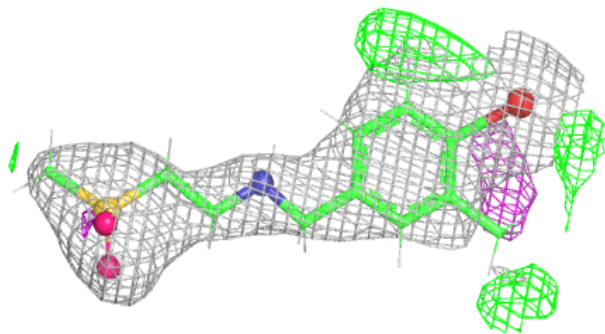
**Electron density around RB7 C 511:**

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

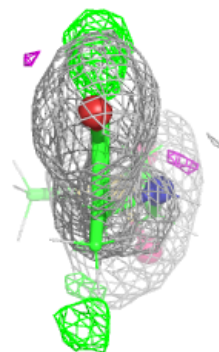
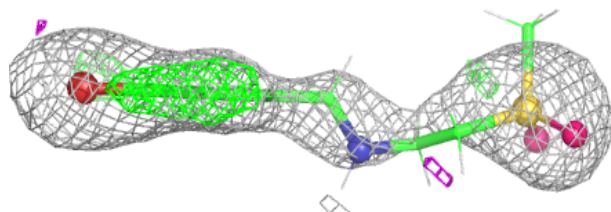
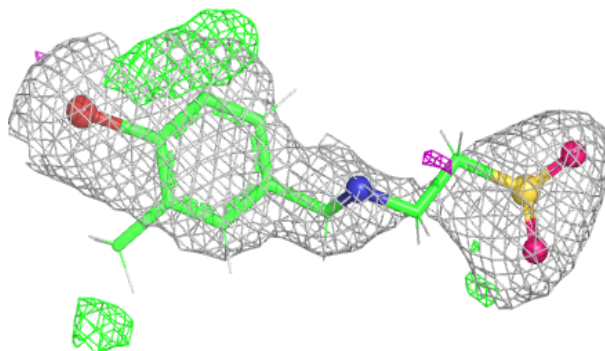


Electron density around RB7 B 506:

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

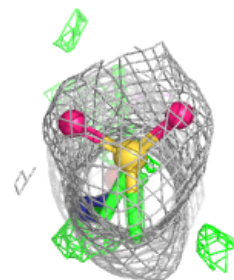
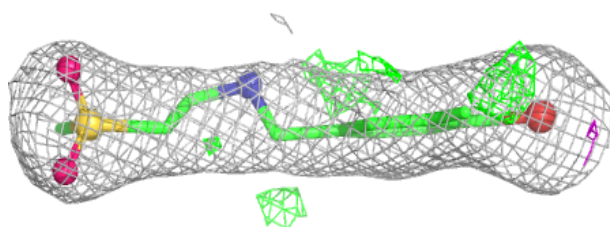
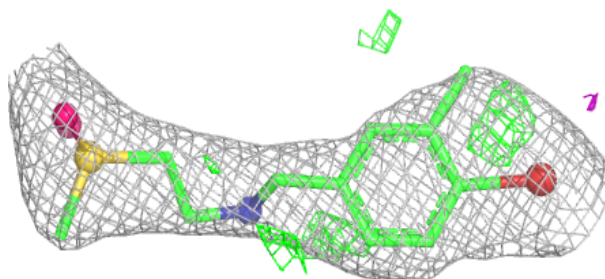
**Electron density around RB7 A 510:**

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

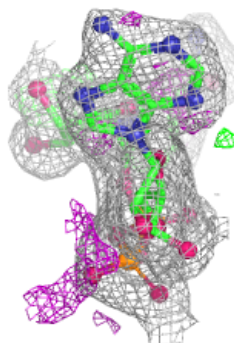
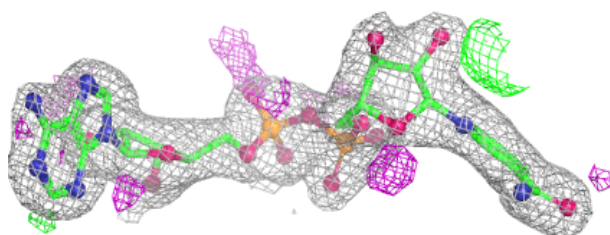
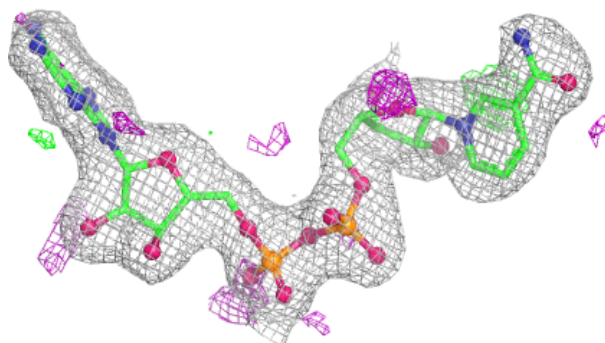


Electron density around RB7 D 509:

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

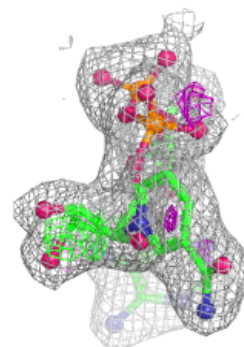
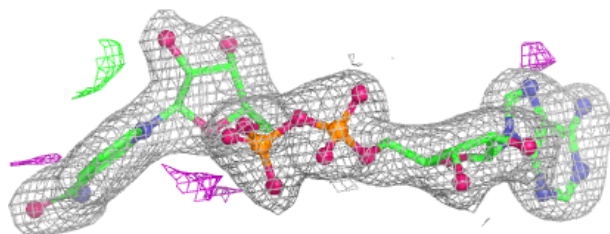
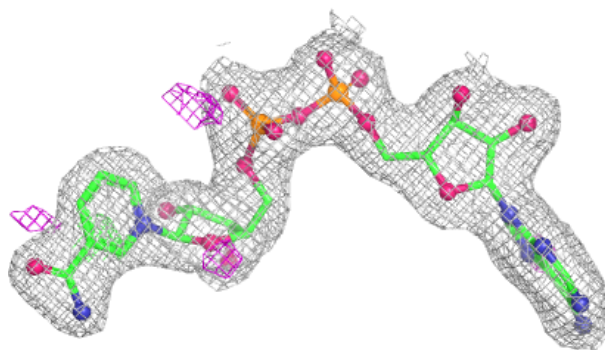
**Electron density around NAD D 501:**

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

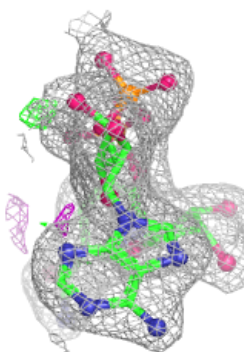
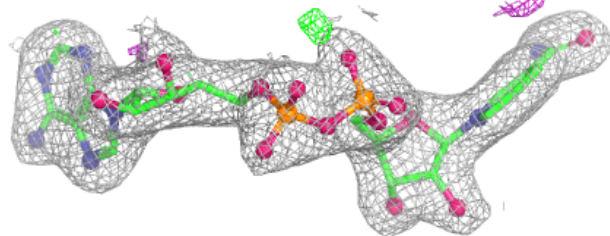
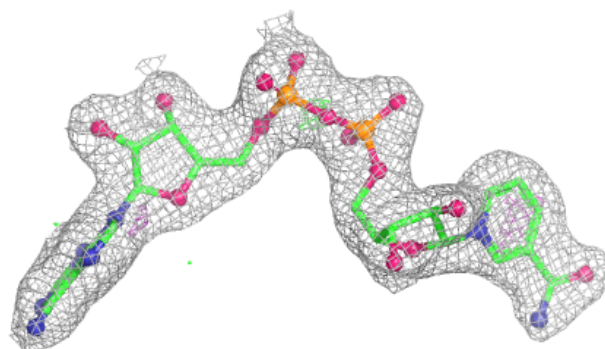


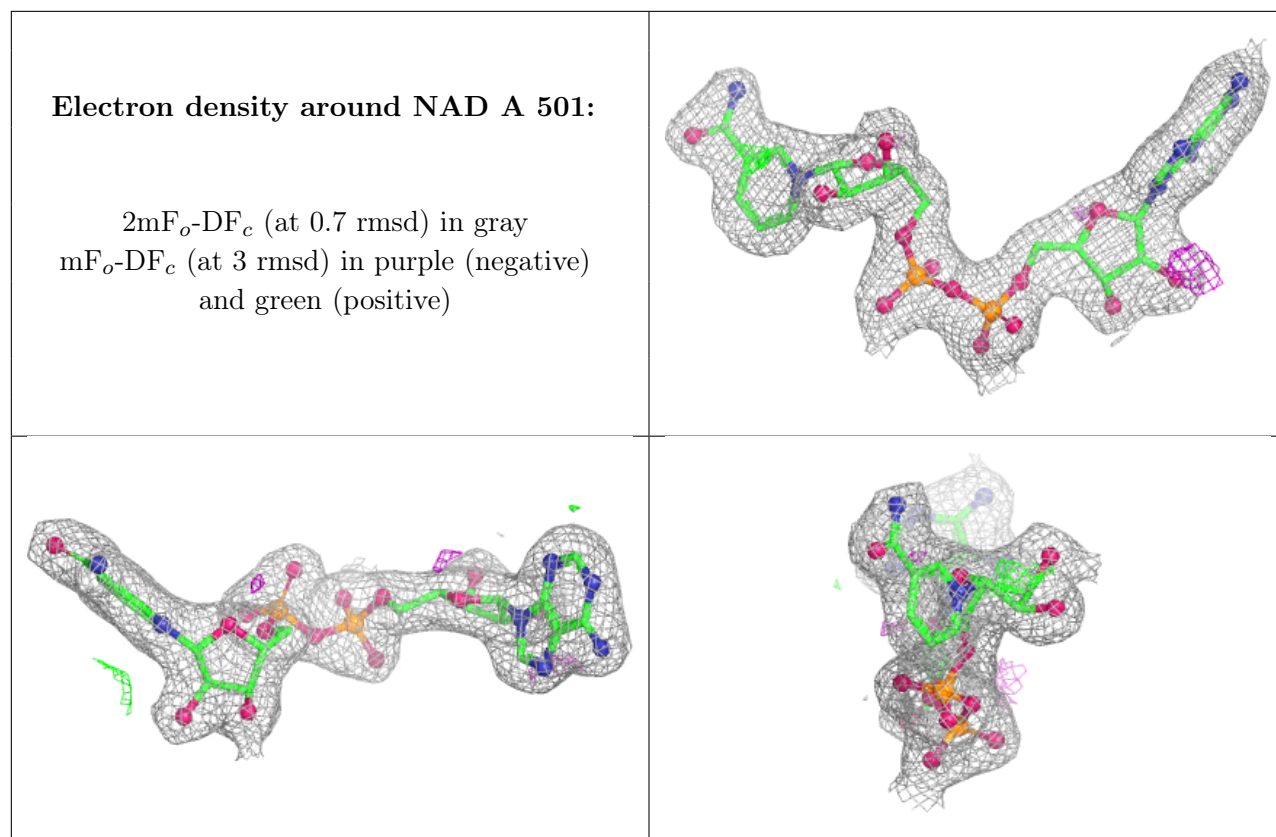
Electron density around NAD B 501:

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

**Electron density around NAD C 501:**

$2mF_o-DF_c$ (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.