



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:56 AM UTC

PDB ID : 1Q51 / pdb_00001q51
Title : Crystal Structure of Mycobacterium tuberculosis MenB in Complex with Acetoacetyl-Coenzyme A, a Key Enzyme in Vitamin K2 Biosynthesis
Authors : Truglio, J.J.; Theis, K.; Feng, Y.; Gajda, R.; Machutta, C.; Tonge, P.J.; Kisker, C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2003-08-05
Resolution : 2.30 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

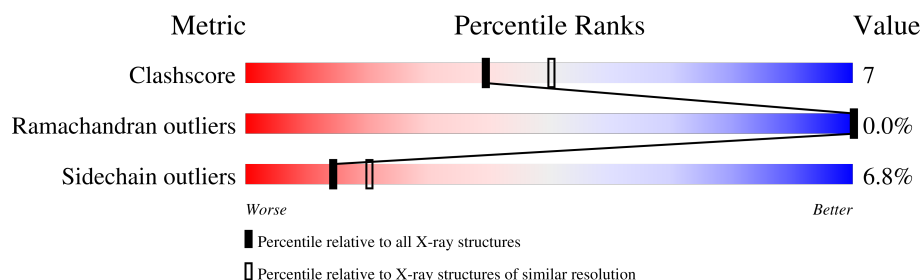
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	67% 18% • 14%
1	B	314	73% 14% •• 11%
1	C	314	73% 12% • 14%
1	D	314	65% 19% • 14%
1	E	314	70% 15% • 14%
1	F	314	69% 15% • 14%
1	G	314	69% 16% • 14%
1	H	314	70% 13% • 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	314	70%15%•14%
1	J	314	69%16%•14%
1	K	314	71%14%•14%
1	L	314	71%14%•14%

2 Entry composition

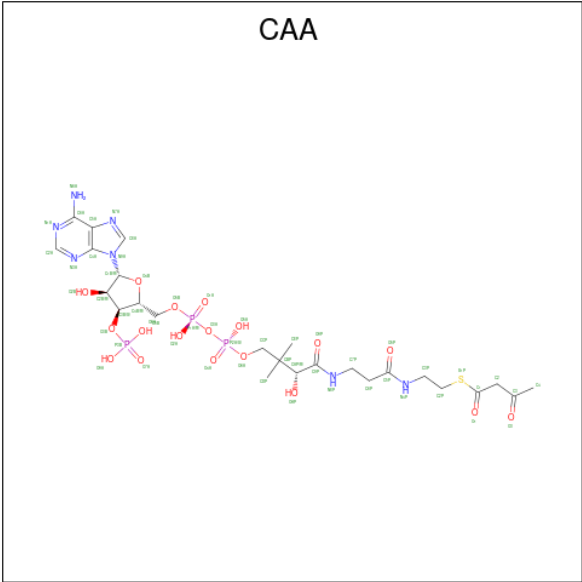
There are 3 unique types of molecules in this entry. The entry contains 26767 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 menB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2136	1355	383	389	9			
1	B	280	Total	C	N	O	S	0	0	0
			2201	1393	398	401	9			
1	C	271	Total	C	N	O	S	0	0	0
			2136	1355	383	389	9			
1	D	271	Total	C	N	O	S	0	0	0
			2136	1355	383	389	9			
1	E	271	Total	C	N	O	S	0	0	0
			2136	1355	383	389	9			
1	F	271	Total	C	N	O	S	0	0	0
			2136	1355	383	389	9			
1	G	271	Total	C	N	O	S	0	0	0
			2136	1355	383	389	9			
1	H	271	Total	C	N	O	S	0	0	0
			2136	1355	383	389	9			
1	I	271	Total	C	N	O	S	0	0	0
			2136	1355	383	389	9			
1	J	271	Total	C	N	O	S	0	0	0
			2136	1355	383	389	9			
1	K	271	Total	C	N	O	S	0	0	0
			2136	1355	383	389	9			
1	L	271	Total	C	N	O	S	0	0	0
			2136	1355	383	389	9			

- Molecule 2 is ACETOACETYL-COENZYME A (CCD ID: CAA) (formula: $C_{25}H_{40}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	K	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		

- Molecule 3 is water.

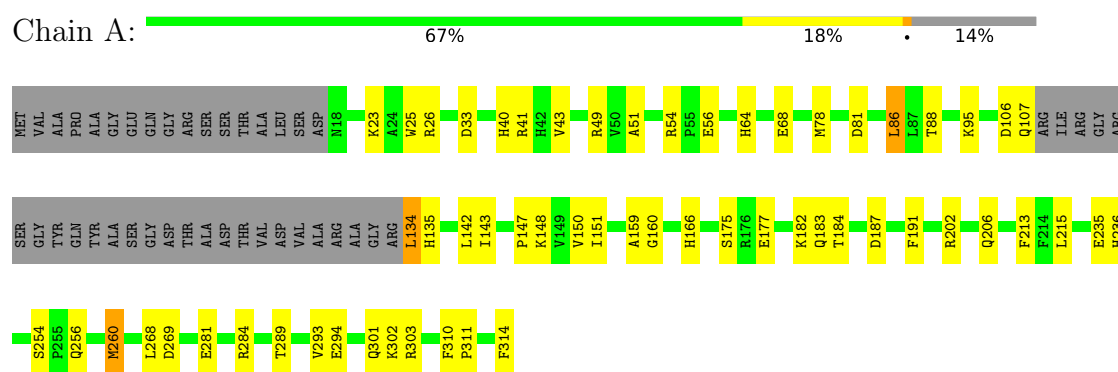
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total 33	O 33	0	0
3	B	35	Total 35	O 35	0	0
3	C	34	Total 34	O 34	0	0
3	D	35	Total 35	O 35	0	0
3	E	39	Total 39	O 39	0	0
3	F	34	Total 34	O 34	0	0
3	G	35	Total 35	O 35	0	0
3	H	34	Total 34	O 34	0	0
3	I	34	Total 34	O 34	0	0
3	J	36	Total 36	O 36	0	0
3	K	36	Total 36	O 36	0	0
3	L	37	Total 37	O 37	0	0

3 Residue-property plots [i](#)

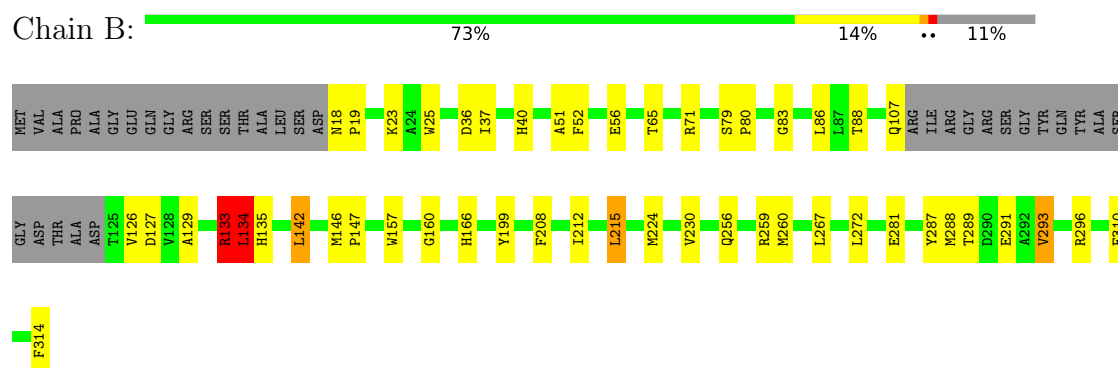
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

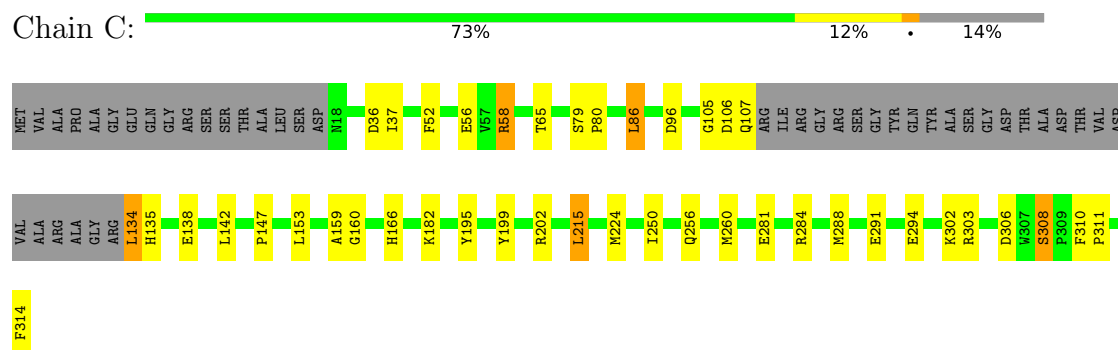
• Molecule 1: menB



• Molecule 1: menB



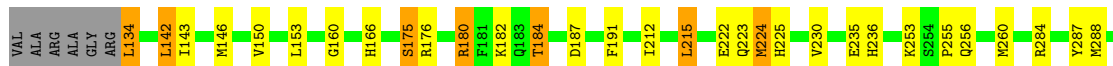
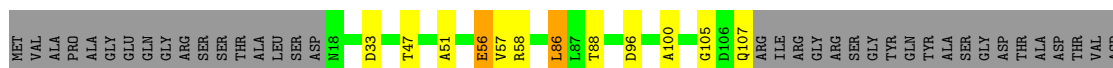
• Molecule 1: menB





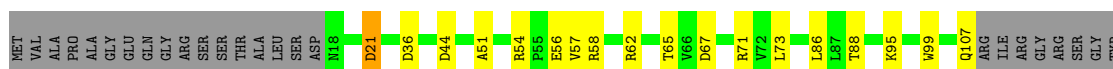
- Molecule 1: menB

Chain H: 70% 13% 14%



- Molecule 1: menB

Chain I: 70% 15% 14%



- Molecule 1: menB

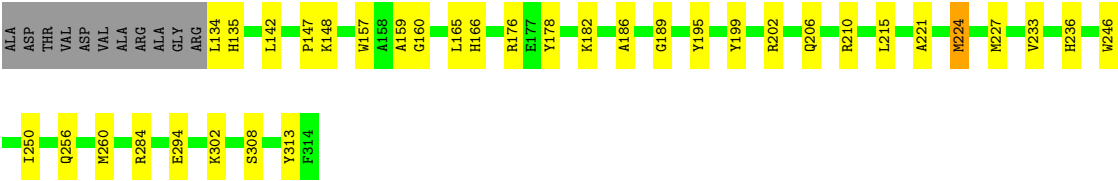
Chain J: 69% 16% 14%



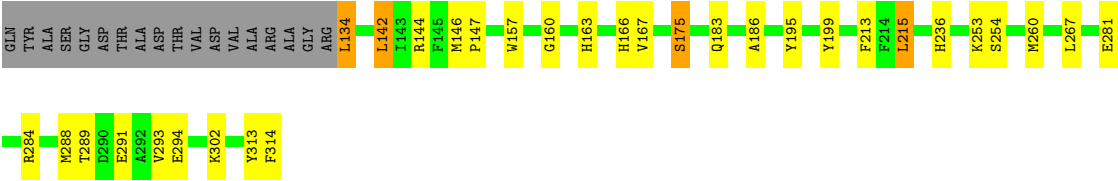
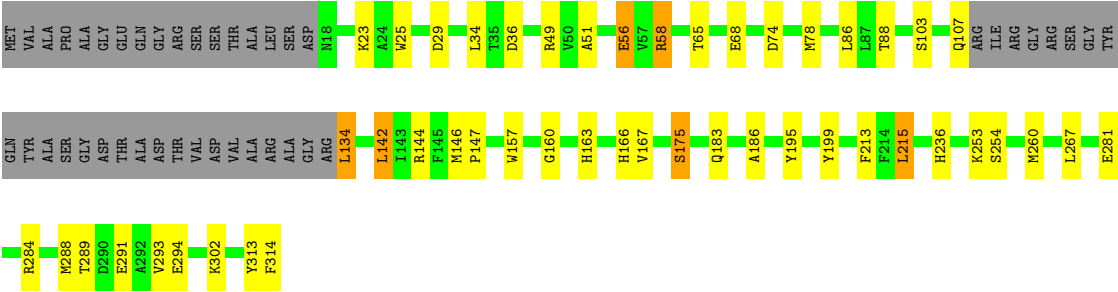
- Molecule 1: menB

Chain K: 71% 14% 14%





• Molecule 1: menB



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.40Å 139.39Å 142.04Å 90.00° 97.31° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30	Depositor
% Data completeness (in resolution range)	99.6 (50.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.202 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26767	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

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: CAA

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	0.85	1/2190 (0.0%)	0.95	1/2969 (0.0%)
1	B	0.83	1/2255 (0.0%)	1.03	6/3057 (0.2%)
1	C	0.84	2/2190 (0.1%)	0.94	0/2969
1	D	0.84	1/2190 (0.0%)	0.98	2/2969 (0.1%)
1	E	0.82	1/2190 (0.0%)	0.95	0/2969
1	F	0.84	2/2190 (0.1%)	0.95	0/2969
1	G	0.82	0/2190	0.96	0/2969
1	H	0.88	2/2190 (0.1%)	0.97	0/2969
1	I	0.82	0/2190	0.95	0/2969
1	J	0.85	2/2190 (0.1%)	0.92	0/2969
1	K	0.82	1/2190 (0.0%)	0.97	0/2969
1	L	0.84	1/2190 (0.0%)	0.94	0/2969
All	All	0.84	14/26345 (0.1%)	0.96	9/35716 (0.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	288	MET	SD-CE	9.12	2.02	1.79
1	H	224	MET	SD-CE	8.77	2.01	1.79
1	H	288	MET	SD-CE	8.25	2.00	1.79
1	J	288	MET	SD-CE	6.73	1.96	1.79
1	F	288	MET	SD-CE	6.52	1.95	1.79
1	J	227	MET	SD-CE	-6.10	1.64	1.79
1	C	288	MET	SD-CE	5.87	1.94	1.79
1	C	224	MET	SD-CE	5.70	1.93	1.79
1	F	146	MET	SD-CE	5.62	1.93	1.79
1	L	288	MET	SD-CE	5.50	1.93	1.79
1	D	288	MET	SD-CE	5.35	1.93	1.79
1	A	260	MET	SD-CE	5.32	1.92	1.79
1	K	88	THR	CA-CB	5.30	1.60	1.53
1	B	288	MET	SD-CE	5.06	1.92	1.79

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	ARG	N-CA-C	10.10	126.28	113.55
1	B	133	ARG	CA-C-N	-6.62	112.65	123.05
1	B	133	ARG	C-N-CA	-6.62	112.65	123.05
1	B	135	HIS	N-CA-C	-6.32	104.44	111.71
1	D	101	PHE	N-CA-C	-5.53	104.11	111.24
1	B	134	LEU	N-CA-C	-5.52	106.13	112.86
1	B	133	ARG	CA-C-O	-5.43	113.42	119.67
1	A	135	HIS	N-CA-C	-5.39	105.57	111.82
1	D	213	PHE	N-CA-C	5.03	117.88	111.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2136	0	2055	32	0
1	B	2201	0	2123	33	0
1	C	2136	0	2055	32	0
1	D	2136	0	2055	46	0
1	E	2136	0	2055	32	0
1	F	2136	0	2055	40	0
1	G	2136	0	2055	32	0
1	H	2136	0	2055	37	0
1	I	2136	0	2055	34	0
1	J	2136	0	2055	28	0
1	K	2136	0	2055	39	0
1	L	2136	0	2055	27	0
2	A	54	0	36	1	0
2	B	54	0	36	2	0
2	C	54	0	36	9	0
2	D	54	0	36	3	0
2	E	54	0	36	1	0
2	F	54	0	36	3	0
2	G	54	0	36	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	54	0	36	3	0
2	I	54	0	36	2	0
2	J	54	0	36	1	0
2	K	54	0	36	8	0
2	L	54	0	36	2	0
3	A	33	0	0	1	0
3	B	35	0	0	0	0
3	C	34	0	0	2	0
3	D	35	0	0	0	0
3	E	39	0	0	0	0
3	F	34	0	0	1	0
3	G	35	0	0	0	0
3	H	34	0	0	1	0
3	I	34	0	0	0	0
3	J	36	0	0	1	0
3	K	36	0	0	0	0
3	L	37	0	0	0	0
All	All	26767	0	25160	345	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 7.

All (345) 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:H:224:MET:SD	1:H:224:MET:CE	2.01	1.48
1:E:288:MET:SD	1:E:288:MET:CE	2.02	1.45
1:D:58:ARG:NH2	1:D:98:GLY:HA3	1.76	1.01
1:K:58:ARG:HG3	1:K:58:ARG:HH11	1.24	0.99
1:K:58:ARG:HH11	1:K:58:ARG:CG	1.87	0.87
1:I:284:ARG:NH2	1:K:134:LEU:HD22	1.95	0.80
1:F:58:ARG:HG3	2:F:506:CAA:H8A	1.64	0.77
1:B:133:ARG:O	1:B:134:LEU:HB2	1.83	0.75
1:C:58:ARG:NH1	2:C:503:CAA:O4A	2.21	0.74
1:G:259:ARG:HD2	1:G:281:GLU:OE1	1.88	0.74
1:G:182:LYS:HG2	1:G:184:THR:HG23	1.71	0.73
1:K:58:ARG:NH1	2:K:500:CAA:O3A	2.16	0.72
1:D:58:ARG:HH21	1:D:98:GLY:HA3	1.51	0.71
1:H:58:ARG:NH2	1:H:96:ASP:OD1	2.24	0.71
1:E:58:ARG:HG3	1:E:100:ALA:HB2	1.71	0.70
1:K:58:ARG:HH12	2:K:500:CAA:P2A	2.14	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ARG:HG2	1:A:49:ARG:HH11	1.57	0.69
1:K:71:ARG:HG2	1:K:71:ARG:HH11	1.59	0.68
1:B:212:ILE:HD13	1:B:224:MET:HE1	1.77	0.67
1:J:290:ASP:O	1:J:293:VAL:HG12	1.95	0.67
1:I:175:SER:OG	1:I:236:HIS:HD2	1.78	0.66
1:A:284:ARG:NH2	1:D:134:LEU:HD22	2.10	0.66
1:D:215:LEU:HD11	1:E:246:TRP:CD2	2.32	0.64
1:E:142:LEU:HD22	1:E:146:MET:HE2	1.78	0.64
1:J:215:LEU:HD22	1:K:250:ILE:HG13	1.77	0.64
1:G:284:ARG:NH2	1:J:134:LEU:HD13	2.13	0.63
1:G:260:MET:HG3	1:I:191:PHE:CZ	2.34	0.62
1:C:58:ARG:HG3	2:C:503:CAA:H8A	1.82	0.62
1:I:284:ARG:HG3	1:I:284:ARG:HH11	1.63	0.62
1:B:291:GLU:HG3	1:B:310:PHE:CD1	2.35	0.62
1:H:47:THR:CG2	1:H:86:LEU:HD22	2.30	0.61
1:B:83:GLY:HA2	1:D:312:ARG:HD3	1.83	0.60
1:H:176:ARG:HH21	1:H:235:GLU:CD	2.09	0.60
1:C:86:LEU:HG	1:C:153:LEU:HD11	1.84	0.60
1:K:157:TRP:CE3	2:K:500:CAA:H133	2.36	0.60
1:I:36:ASP:HB3	1:I:65:THR:HG23	1.84	0.59
1:A:147:PRO:HG3	1:E:314:PHE:HA	1.82	0.59
1:G:269:ASP:HB3	1:J:272:LEU:HD12	1.85	0.59
1:K:107:GLN:NE2	2:K:500:CAA:S1P	2.76	0.59
1:K:157:TRP:CZ3	2:K:500:CAA:H133	2.38	0.59
1:D:58:ARG:HH22	1:D:98:GLY:HA3	1.63	0.58
1:C:260:MET:SD	1:C:281:GLU:HB3	2.43	0.58
1:E:260:MET:SD	1:E:281:GLU:HB3	2.44	0.57
1:K:186:ALA:HB3	1:L:253:LYS:HD2	1.87	0.57
1:G:284:ARG:HH11	1:G:284:ARG:HG3	1.70	0.57
1:L:289:THR:O	1:L:293:VAL:HG23	2.05	0.56
1:G:314:PHE:HA	1:K:147:PRO:HG3	1.87	0.56
1:I:176:ARG:HH21	1:I:235:GLU:CD	2.13	0.56
1:B:212:ILE:CD1	1:B:224:MET:HE1	2.35	0.56
1:K:58:ARG:CG	1:K:58:ARG:NH1	2.56	0.56
1:A:54:ARG:NH1	1:A:106:ASP:OD2	2.35	0.56
1:A:260:MET:SD	1:A:281:GLU:HB3	2.45	0.56
1:B:314:PHE:HA	1:D:147:PRO:HG3	1.85	0.56
1:F:142:LEU:HD22	1:F:146:MET:HE2	1.86	0.56
1:D:43:VAL:HG23	1:D:44:ASP:OD1	2.05	0.56
1:G:175:SER:OG	1:G:236:HIS:HD2	1.89	0.56
1:D:175:SER:OG	1:D:236:HIS:HD2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:GLY:HA3	2:D:504:CAA:H31	1.88	0.55
1:K:224:MET:SD	1:K:227:MET:HE3	2.46	0.55
1:D:211:GLU:HB2	1:E:231:ASN:ND2	2.20	0.55
1:H:88:THR:HB	1:H:153:LEU:HB2	1.87	0.55
1:F:66:VAL:HG11	1:F:135:HIS:HB3	1.88	0.55
1:C:134:LEU:HD13	1:E:284:ARG:NH2	2.22	0.55
1:D:76:ALA:O	1:D:148:LYS:HE3	2.05	0.54
1:B:134:LEU:HD22	1:F:284:ARG:NH2	2.22	0.54
1:K:36:ASP:HB3	1:K:65:THR:HG23	1.88	0.54
1:F:160:GLY:HA3	2:F:506:CAA:H31	1.90	0.54
1:I:224:MET:SD	1:I:227:MET:HE3	2.48	0.53
1:C:284:ARG:HG3	1:C:284:ARG:HH11	1.74	0.53
1:C:106:ASP:OD1	2:C:503:CAA:H2A	2.08	0.53
1:C:160:GLY:HA3	2:C:503:CAA:H31	1.91	0.53
1:F:177:GLU:HA	1:H:180:ARG:HH12	1.73	0.53
1:J:256:GLN:O	1:J:260:MET:HG2	2.08	0.53
1:K:221:ALA:HB1	1:K:233:VAL:HG22	1.90	0.53
1:L:260:MET:SD	1:L:281:GLU:HB3	2.48	0.53
1:D:224:MET:HB3	1:D:230:VAL:HG23	1.91	0.53
1:B:129:ALA:HB2	1:C:311:PRO:HB2	1.90	0.53
1:C:314:PHE:HA	1:F:147:PRO:HG3	1.91	0.52
1:F:303:ARG:HB2	1:F:304:PRO:HD2	1.90	0.52
1:B:289:THR:O	1:B:293:VAL:HG23	2.09	0.52
1:E:99:TRP:CE2	1:E:236:HIS:HE1	2.27	0.52
1:L:142:LEU:HD22	1:L:146:MET:HE2	1.91	0.52
1:F:67:ASP:O	1:F:71:ARG:HG3	2.08	0.52
1:F:177:GLU:O	1:H:180:ARG:NH1	2.43	0.52
1:B:272:LEU:HD12	1:F:269:ASP:HB3	1.92	0.52
1:F:159:ALA:HA	1:F:182:LYS:O	2.10	0.52
1:I:314:PHE:HA	1:L:147:PRO:HG3	1.92	0.52
1:K:160:GLY:HA3	2:K:500:CAA:H31	1.91	0.52
1:A:289:THR:O	1:A:293:VAL:HG23	2.10	0.51
1:F:36:ASP:HB3	1:F:65:THR:HG23	1.92	0.51
1:E:293:VAL:HA	1:E:296:ARG:NH1	2.25	0.51
1:H:314:PHE:HA	1:J:147:PRO:HG3	1.91	0.51
1:I:67:ASP:OD1	1:I:135:HIS:CD2	2.63	0.51
1:L:36:ASP:HB3	1:L:65:THR:HG23	1.92	0.51
1:C:58:ARG:HH11	2:C:503:CAA:P2A	2.33	0.51
1:K:195:TYR:O	1:K:199:TYR:HB3	2.10	0.51
1:E:86:LEU:HG	1:E:153:LEU:HD11	1.93	0.51
1:D:260:MET:SD	1:D:281:GLU:HB3	2.51	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:TRP:CZ3	2:G:507:CAA:H133	2.46	0.51
1:H:224:MET:CE	1:H:224:MET:CG	2.89	0.51
1:I:54:ARG:NH1	1:I:62:ARG:HG2	2.25	0.51
1:G:183:GLN:HG2	1:G:213:PHE:CZ	2.47	0.50
1:J:58:ARG:HG3	1:J:100:ALA:HB2	1.93	0.50
1:H:58:ARG:HD3	1:H:100:ALA:HB2	1.92	0.50
1:J:36:ASP:HB3	1:J:65:THR:HG23	1.93	0.50
1:A:25:TRP:HB3	1:A:40:HIS:HB3	1.93	0.50
1:E:256:GLN:O	1:E:260:MET:HG2	2.12	0.50
1:I:284:ARG:HH22	1:K:134:LEU:HD22	1.75	0.50
1:B:147:PRO:HG3	1:D:314:PHE:HA	1.94	0.50
1:A:269:ASP:HB3	1:D:272:LEU:HD12	1.92	0.50
1:C:36:ASP:HB3	1:C:65:THR:HG23	1.93	0.50
1:H:182:LYS:HG2	1:H:184:THR:HG23	1.93	0.50
1:H:160:GLY:HA3	2:H:508:CAA:H31	1.94	0.49
1:H:287:TYR:O	1:H:296:ARG:NH2	2.44	0.49
1:I:51:ALA:HA	1:I:88:THR:O	2.13	0.49
1:H:142:LEU:HD22	1:H:146:MET:HE2	1.93	0.49
1:A:86:LEU:HD12	1:A:151:ILE:HB	1.93	0.49
1:C:147:PRO:HG3	1:F:314:PHE:HA	1.95	0.49
1:D:58:ARG:HH21	1:D:98:GLY:CA	2.24	0.49
1:H:191:PHE:CZ	1:I:260:MET:HG3	2.47	0.49
1:I:142:LEU:HD22	1:I:146:MET:HE2	1.94	0.49
1:H:175:SER:OG	1:H:236:HIS:HD2	1.95	0.49
1:D:250:ILE:HG13	1:F:215:LEU:HD22	1.94	0.49
1:D:182:LYS:HG2	1:D:184:THR:HG23	1.94	0.49
1:D:250:ILE:HG13	1:F:215:LEU:CD2	2.43	0.49
1:C:58:ARG:NH1	2:C:503:CAA:P2A	2.86	0.49
1:E:224:MET:HB3	1:E:230:VAL:HG23	1.93	0.49
1:H:313:TYR:HB3	1:J:284:ARG:CZ	2.43	0.48
1:J:184:THR:O	1:J:187:ASP:HB2	2.13	0.48
1:A:26:ARG:HG2	1:A:43:VAL:HG12	1.94	0.48
1:B:160:GLY:HA3	2:B:502:CAA:H31	1.95	0.48
1:C:134:LEU:HD13	1:E:284:ARG:HH22	1.78	0.48
1:H:255:PRO:HD2	1:J:291:GLU:OE1	2.14	0.48
1:B:36:ASP:HB3	1:B:65:THR:HG23	1.95	0.48
1:F:175:SER:CB	1:F:236:HIS:HD2	2.27	0.48
1:F:260:MET:SD	1:F:281:GLU:HB3	2.54	0.48
1:F:259:ARG:HD2	1:F:281:GLU:OE1	2.12	0.48
1:E:160:GLY:HA3	2:E:505:CAA:H31	1.96	0.47
1:G:231:ASN:ND2	1:I:211:GLU:HB2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:189:GLY:HA2	1:L:254:SER:CB	2.44	0.47
1:L:183:GLN:HG2	1:L:213:PHE:CE2	2.49	0.47
1:D:51:ALA:HA	1:D:88:THR:O	2.14	0.47
1:D:186:ALA:HB3	1:E:253:LYS:HD3	1.95	0.47
1:I:284:ARG:HG3	1:I:284:ARG:NH1	2.28	0.47
1:J:303:ARG:HB2	1:J:304:PRO:HD2	1.96	0.47
1:A:143:ILE:HG23	1:A:150:VAL:HG21	1.96	0.47
1:B:51:ALA:HA	1:B:88:THR:O	2.14	0.47
1:F:222:GLU:OE1	1:F:226:GLN:NE2	2.46	0.47
1:C:135:HIS:O	1:C:138:GLU:HB2	2.15	0.47
1:K:159:ALA:HA	1:K:182:LYS:O	2.15	0.47
1:F:56:GLU:CD	1:F:56:GLU:H	2.23	0.47
1:H:143:ILE:HG23	1:H:150:VAL:HG21	1.97	0.47
1:J:202:ARG:HH11	1:J:269:ASP:CG	2.23	0.47
3:C:537:HOH:O	1:F:80:PRO:HA	2.14	0.46
1:F:135:HIS:O	1:F:138:GLU:HB2	2.15	0.46
1:A:310:PHE:HA	1:A:311:PRO:HD3	1.80	0.46
1:D:57:VAL:HG12	2:D:504:CAA:H1B	1.96	0.46
1:K:58:ARG:NH1	2:K:500:CAA:P2A	2.85	0.46
1:D:256:GLN:O	1:D:260:MET:HG2	2.16	0.46
1:F:58:ARG:NH2	1:F:96:ASP:OD1	2.47	0.46
1:F:136:ILE:HD11	1:F:165:LEU:HD11	1.97	0.46
1:L:51:ALA:HA	1:L:88:THR:O	2.14	0.46
1:K:56:GLU:H	1:K:56:GLU:HG3	1.28	0.46
1:C:58:ARG:NH2	1:C:96:ASP:OD2	2.48	0.46
1:G:284:ARG:CZ	1:K:313:TYR:HB3	2.46	0.46
1:E:310:PHE:HA	1:E:311:PRO:HD3	1.76	0.46
1:H:284:ARG:NH2	1:L:134:LEU:HD13	2.31	0.46
1:F:58:ARG:HG3	2:F:506:CAA:C8A	2.42	0.46
1:G:210:ARG:HB3	1:G:214:PHE:CE1	2.50	0.46
1:C:256:GLN:O	1:C:260:MET:HG2	2.16	0.46
1:D:180:ARG:NH1	1:G:177:GLU:O	2.49	0.46
1:G:254:SER:CB	1:I:189:GLY:HA2	2.46	0.46
1:L:163:HIS:O	1:L:167:VAL:HG23	2.16	0.46
1:B:260:MET:SD	1:B:281:GLU:HB3	2.56	0.45
1:C:291:GLU:OE1	1:F:254:SER:OG	2.28	0.45
1:G:157:TRP:CE3	2:G:507:CAA:H133	2.51	0.45
1:A:78:MET:HG2	1:E:314:PHE:CE2	2.51	0.45
1:G:195:TYR:O	1:G:199:TYR:HB3	2.16	0.45
1:A:64:HIS:O	1:A:68:GLU:HG3	2.17	0.45
1:B:147:PRO:HB2	1:B:259:ARG:CG	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:179:ALA:C	1:I:180:ARG:HG2	2.41	0.45
1:A:33:ASP:OD1	1:A:33:ASP:N	2.45	0.45
1:H:187:ASP:OD1	1:I:253:LYS:NZ	2.40	0.45
1:H:215:LEU:HB2	3:H:511:HOH:O	2.16	0.45
1:I:58:ARG:HG3	2:I:509:CAA:H8A	1.97	0.45
1:I:134:LEU:HD22	1:K:284:ARG:NH2	2.31	0.45
1:B:25:TRP:HB3	1:B:40:HIS:HB3	1.99	0.45
1:D:289:THR:O	1:D:293:VAL:HG23	2.16	0.45
1:J:39:TYR:CD2	1:J:72:VAL:HG13	2.52	0.45
1:L:195:TYR:O	1:L:199:TYR:HB3	2.17	0.45
1:E:221:ALA:HB1	1:E:233:VAL:HG22	1.98	0.45
1:H:175:SER:CB	1:H:236:HIS:HD2	2.30	0.45
1:H:56:GLU:CD	1:H:56:GLU:H	2.24	0.45
1:J:159:ALA:HA	1:J:182:LYS:O	2.16	0.45
1:A:64:HIS:NE2	1:A:68:GLU:OE2	2.50	0.45
1:C:58:ARG:NH1	2:C:503:CAA:O3A	2.50	0.45
1:G:58:ARG:HD3	2:G:507:CAA:H52A	1.99	0.44
1:I:284:ARG:CZ	1:L:313:TYR:HB3	2.47	0.44
1:J:37:ILE:HD11	1:J:65:THR:HG22	2.00	0.44
1:E:293:VAL:HA	1:E:296:ARG:HH12	1.81	0.44
1:B:287:TYR:O	1:B:296:ARG:NH2	2.45	0.44
1:J:215:LEU:CD2	1:K:250:ILE:HG13	2.47	0.44
1:A:284:ARG:HH22	1:D:134:LEU:HD22	1.80	0.44
1:B:134:LEU:HD22	1:F:284:ARG:HH22	1.82	0.44
1:J:160:GLY:HA3	2:J:510:CAA:H31	2.00	0.44
1:A:41:ARG:NH1	1:A:81:ASP:OD2	2.51	0.44
1:K:105:GLY:H	2:K:500:CAA:C1	2.30	0.44
1:L:175:SER:OG	1:L:236:HIS:HD2	2.01	0.44
1:E:25:TRP:CH2	1:E:49:ARG:HB2	2.53	0.44
1:H:310:PHE:HA	1:H:311:PRO:HD3	1.81	0.44
1:E:146:MET:O	1:E:262:LYS:HE2	2.17	0.43
1:J:310:PHE:HA	1:J:311:PRO:HD3	1.80	0.43
1:A:301:GLN:OE1	1:A:303:ARG:HD3	2.17	0.43
1:A:268:LEU:HD23	1:E:268:LEU:HD23	2.00	0.43
1:G:160:GLY:HA3	2:G:507:CAA:H31	2.00	0.43
1:B:256:GLN:O	1:B:260:MET:HG2	2.18	0.43
1:F:256:GLN:NE2	1:F:285:LEU:CD2	2.81	0.43
1:G:289:THR:O	1:G:293:VAL:HG23	2.19	0.43
1:J:39:TYR:CG	1:J:72:VAL:HG13	2.53	0.43
1:J:260:MET:SD	1:J:281:GLU:HB3	2.59	0.43
1:I:160:GLY:HA2	1:I:183:GLN:OE1	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:250:ILE:HG13	1:L:215:LEU:HD22	2.01	0.43
1:A:206:GLN:HG3	1:B:199:TYR:CE2	2.54	0.43
1:C:79:SER:HA	1:C:80:PRO:HD3	1.81	0.43
1:D:212:ILE:CD1	1:D:224:MET:HE1	2.49	0.43
1:H:256:GLN:O	1:H:260:MET:HG2	2.18	0.43
1:L:157:TRP:CZ3	2:L:511:CAA:H133	2.54	0.43
1:A:184:THR:O	1:A:187:ASP:HB2	2.18	0.43
1:F:86:LEU:HG	1:F:153:LEU:HD11	2.01	0.43
1:G:183:GLN:HG2	1:G:213:PHE:CE2	2.53	0.43
1:G:284:ARG:HG3	1:G:284:ARG:NH1	2.32	0.43
1:G:308:SER:N	1:G:309:PRO:CD	2.82	0.43
1:J:215:LEU:HD11	1:K:246:TRP:CD2	2.54	0.43
1:K:206:GLN:O	1:K:210:ARG:HG3	2.18	0.43
1:H:58:ARG:NH1	2:H:508:CAA:O4A	2.52	0.43
1:J:83:GLY:O	1:J:148:LYS:HB2	2.19	0.43
1:L:56:GLU:H	1:L:56:GLU:CD	2.27	0.43
1:C:105:GLY:H	2:C:503:CAA:C1	2.32	0.43
1:C:306:ASP:OD1	1:C:308:SER:OG	2.35	0.43
1:E:79:SER:HA	1:E:80:PRO:HD3	1.84	0.43
1:G:62:ARG:HB2	1:G:63:PRO:HD2	2.00	0.43
1:G:159:ALA:HA	1:G:182:LYS:O	2.18	0.43
1:L:160:GLY:HA3	2:L:511:CAA:H31	2.00	0.43
1:B:291:GLU:OE1	1:D:255:PRO:HD2	2.18	0.42
1:D:58:ARG:NH1	2:D:504:CAA:O4A	2.52	0.42
1:H:51:ALA:HA	1:H:88:THR:O	2.19	0.42
1:H:222:GLU:OE1	1:H:225:HIS:HD2	2.02	0.42
1:K:71:ARG:HH11	1:K:71:ARG:CG	2.30	0.42
1:A:160:GLY:HA3	2:A:501:CAA:H31	2.01	0.42
1:E:159:ALA:HA	1:E:182:LYS:O	2.18	0.42
1:G:187:ASP:OD1	1:H:253:LYS:HD3	2.19	0.42
1:I:21:ASP:OD1	1:I:21:ASP:O	2.37	0.42
1:K:176:ARG:HB2	1:K:233:VAL:CG1	2.49	0.42
1:A:51:ALA:HA	1:A:88:THR:O	2.19	0.42
1:E:56:GLU:H	1:E:56:GLU:CD	2.26	0.42
1:A:191:PHE:CE2	1:B:260:MET:HG3	2.55	0.42
1:A:256:GLN:HB2	1:E:291:GLU:CD	2.45	0.42
1:B:37:ILE:HD13	1:B:52:PHE:HA	2.02	0.42
1:K:256:GLN:O	1:K:260:MET:HG2	2.20	0.42
1:E:45:ASP:OD1	1:E:45:ASP:N	2.51	0.42
1:J:51:ALA:HA	1:J:88:THR:O	2.20	0.42
1:J:253:LYS:HD2	1:L:186:ALA:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:PHE:O	1:C:134:LEU:HD22	2.20	0.42
1:B:79:SER:HA	1:B:80:PRO:HD3	1.87	0.42
1:D:175:SER:OG	1:D:236:HIS:CD2	2.71	0.42
1:E:51:ALA:HA	1:E:88:THR:O	2.20	0.42
1:F:25:TRP:CH2	1:F:49:ARG:HB2	2.55	0.42
1:G:250:ILE:HG13	1:I:215:LEU:HD22	2.01	0.42
1:K:165:LEU:HA	1:K:165:LEU:HD23	1.82	0.42
1:B:215:LEU:HD22	1:C:250:ILE:HG13	2.02	0.42
1:D:34:LEU:HA	1:D:68:GLU:OE2	2.19	0.42
1:D:310:PHE:HA	1:D:311:PRO:HD3	1.86	0.42
1:L:25:TRP:CH2	1:L:49:ARG:HB2	2.55	0.42
1:A:159:ALA:HA	1:A:182:LYS:O	2.19	0.42
1:B:208:PHE:O	1:B:212:ILE:HG13	2.20	0.42
1:I:160:GLY:HA3	2:I:509:CAA:H31	2.01	0.42
1:C:159:ALA:HA	1:C:182:LYS:O	2.20	0.42
1:D:18:ASN:HA	1:D:19:PRO:HD3	1.88	0.42
1:E:195:TYR:O	1:E:199:TYR:HB3	2.20	0.42
1:I:256:GLN:HB3	1:L:291:GLU:OE1	2.20	0.42
1:K:176:ARG:HB2	1:K:233:VAL:HG13	2.02	0.42
3:A:522:HOH:O	1:B:256:GLN:HB3	2.20	0.41
1:C:310:PHE:HA	1:C:311:PRO:HD3	1.73	0.41
1:D:159:ALA:HA	1:D:182:LYS:O	2.20	0.41
1:F:58:ARG:NH2	1:F:98:GLY:HA3	2.35	0.41
1:I:202:ARG:NH1	1:I:269:ASP:OD1	2.53	0.41
1:K:99:TRP:CZ2	1:K:236:HIS:HE1	2.37	0.41
1:A:134:LEU:HD22	1:D:284:ARG:NH2	2.34	0.41
1:D:308:SER:N	1:D:309:PRO:CD	2.83	0.41
1:F:184:THR:O	1:F:187:ASP:HB2	2.20	0.41
1:G:224:MET:HB3	1:G:230:VAL:HG23	2.01	0.41
1:K:51:ALA:HA	1:K:88:THR:O	2.20	0.41
1:E:99:TRP:CZ2	1:E:236:HIS:HE1	2.38	0.41
1:F:308:SER:N	1:F:309:PRO:CD	2.83	0.41
1:J:173:LEU:HD13	1:J:242:VAL:HG12	2.01	0.41
1:F:215:LEU:HB2	3:F:509:HOH:O	2.21	0.41
1:K:66:VAL:HG11	1:K:135:HIS:HB3	2.02	0.41
1:K:178:TYR:HD1	1:K:236:HIS:CD2	2.38	0.41
1:B:224:MET:HB3	1:B:230:VAL:HG23	2.03	0.41
1:D:176:ARG:HH11	1:D:176:ARG:HG2	1.86	0.41
1:I:267:LEU:C	1:I:267:LEU:HD23	2.45	0.41
1:B:157:TRP:CE3	2:B:502:CAA:H133	2.56	0.41
1:C:80:PRO:O	1:F:312:ARG:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ASP:HA	2:C:503:CAA:N1A	2.36	0.41
1:D:93:SER:HA	1:D:94:PRO:HD3	1.91	0.41
1:H:284:ARG:HH22	1:L:134:LEU:HD13	1.83	0.41
1:B:267:LEU:C	1:B:267:LEU:HD23	2.46	0.41
1:C:37:ILE:HD13	1:C:52:PHE:HA	2.03	0.41
1:G:276:GLN:HG3	3:J:516:HOH:O	2.21	0.41
1:G:306:ASP:OD1	1:G:308:SER:OG	2.27	0.41
1:H:212:ILE:HG12	1:H:224:MET:HE1	2.03	0.41
1:H:224:MET:HB3	1:H:230:VAL:HG23	2.03	0.41
1:I:73:LEU:HB2	1:I:142:LEU:HD13	2.03	0.41
1:K:77:ARG:HA	1:K:148:LYS:HE3	2.02	0.41
1:A:183:GLN:HG2	1:A:213:PHE:CZ	2.56	0.41
1:H:58:ARG:HH22	1:H:96:ASP:CG	2.29	0.41
1:I:147:PRO:HG3	1:L:314:PHE:HA	2.03	0.41
1:L:58:ARG:HB3	1:L:103:SER:HB3	2.03	0.41
1:L:74:ASP:O	1:L:78:MET:HG3	2.21	0.41
1:G:62:ARG:HB2	1:G:63:PRO:CD	2.51	0.40
1:I:99:TRP:CZ2	1:I:236:HIS:HE1	2.39	0.40
1:A:182:LYS:HG2	1:A:184:THR:HG23	2.03	0.40
1:C:195:TYR:O	1:C:199:TYR:HB3	2.21	0.40
1:D:29:ASP:OD1	1:D:29:ASP:N	2.54	0.40
1:D:36:ASP:HB3	1:D:65:THR:HG23	2.02	0.40
1:G:86:LEU:HG	1:G:153:LEU:HD11	2.04	0.40
1:H:105:GLY:H	2:H:508:CAA:C1	2.34	0.40
1:H:134:LEU:HD22	1:L:284:ARG:HH22	1.86	0.40
1:D:69:LEU:HG	1:D:73:LEU:CD1	2.51	0.40
1:D:79:SER:HA	1:D:80:PRO:HD3	1.83	0.40
1:F:192:ASP:OD1	1:F:192:ASP:C	2.65	0.40
1:I:175:SER:OG	1:I:236:HIS:CD2	2.66	0.40
1:J:267:LEU:HD23	1:J:267:LEU:C	2.45	0.40
1:A:175:SER:OG	1:A:236:HIS:HD2	2.04	0.40
1:B:18:ASN:HA	1:B:19:PRO:HD3	1.93	0.40
1:B:142:LEU:HD22	1:B:146:MET:HE2	2.03	0.40
1:D:25:TRP:CH2	1:D:244:LEU:HD21	2.56	0.40
1:D:267:LEU:C	1:D:267:LEU:HD23	2.46	0.40
1:L:34:LEU:HA	1:L:68:GLU:OE2	2.21	0.40
1:C:215:LEU:HB2	3:C:506:HOH:O	2.21	0.40
1:D:246:TRP:CD2	1:F:215:LEU:HD11	2.56	0.40
1:E:39:TYR:CD2	1:E:72:VAL:HG13	2.57	0.40
1:F:67:ASP:OD1	1:F:135:HIS:CD2	2.75	0.40
1:F:176:ARG:NH1	1:H:223:GLN:OE1	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:183:GLN:HG2	1:I:213:PHE:CE2	2.57	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	267/314 (85%)	260 (97%)	7 (3%)	0	100	100
1	B	276/314 (88%)	266 (96%)	10 (4%)	0	100	100
1	C	267/314 (85%)	259 (97%)	8 (3%)	0	100	100
1	D	267/314 (85%)	260 (97%)	7 (3%)	0	100	100
1	E	267/314 (85%)	259 (97%)	8 (3%)	0	100	100
1	F	267/314 (85%)	260 (97%)	7 (3%)	0	100	100
1	G	267/314 (85%)	261 (98%)	6 (2%)	0	100	100
1	H	267/314 (85%)	259 (97%)	8 (3%)	0	100	100
1	I	267/314 (85%)	260 (97%)	7 (3%)	0	100	100
1	J	267/314 (85%)	260 (97%)	7 (3%)	0	100	100
1	K	267/314 (85%)	259 (97%)	8 (3%)	0	100	100
1	L	267/314 (85%)	260 (97%)	6 (2%)	1 (0%)	30	38
All	All	3213/3768 (85%)	3123 (97%)	89 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	267	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	217/247 (88%)	201 (93%)	16 (7%)	13	17
1	B	223/247 (90%)	210 (94%)	13 (6%)	18	26
1	C	217/247 (88%)	204 (94%)	13 (6%)	17	25
1	D	217/247 (88%)	203 (94%)	14 (6%)	15	22
1	E	217/247 (88%)	206 (95%)	11 (5%)	21	32
1	F	217/247 (88%)	203 (94%)	14 (6%)	15	22
1	G	217/247 (88%)	199 (92%)	18 (8%)	10	14
1	H	217/247 (88%)	202 (93%)	15 (7%)	14	20
1	I	217/247 (88%)	198 (91%)	19 (9%)	9	12
1	J	217/247 (88%)	200 (92%)	17 (8%)	11	16
1	K	217/247 (88%)	203 (94%)	14 (6%)	15	22
1	L	217/247 (88%)	203 (94%)	14 (6%)	15	22
All	All	2610/2964 (88%)	2432 (93%)	178 (7%)	14	20

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	56	GLU
1	A	86	LEU
1	A	95	LYS
1	A	107	GLN
1	A	134	LEU
1	A	142	LEU
1	A	148	LYS
1	A	166	HIS
1	A	177	GLU
1	A	202	ARG
1	A	215	LEU
1	A	235	GLU
1	A	254	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	294	GLU
1	A	302	LYS
1	B	23	LYS
1	B	56	GLU
1	B	71	ARG
1	B	86	LEU
1	B	107	GLN
1	B	126	VAL
1	B	127	ASP
1	B	133	ARG
1	B	134	LEU
1	B	142	LEU
1	B	166	HIS
1	B	215	LEU
1	B	293	VAL
1	C	56	GLU
1	C	58	ARG
1	C	86	LEU
1	C	107	GLN
1	C	134	LEU
1	C	142	LEU
1	C	166	HIS
1	C	202	ARG
1	C	215	LEU
1	C	294	GLU
1	C	302	LYS
1	C	303	ARG
1	C	308	SER
1	D	44	ASP
1	D	56	GLU
1	D	57	VAL
1	D	58	ARG
1	D	86	LEU
1	D	95	LYS
1	D	134	LEU
1	D	142	LEU
1	D	166	HIS
1	D	215	LEU
1	D	294	GLU
1	D	302	LYS
1	D	308	SER
1	D	312	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	58	ARG
1	E	86	LEU
1	E	107	GLN
1	E	134	LEU
1	E	142	LEU
1	E	166	HIS
1	E	175	SER
1	E	184	THR
1	E	215	LEU
1	E	294	GLU
1	E	302	LYS
1	F	56	GLU
1	F	58	ARG
1	F	86	LEU
1	F	107	GLN
1	F	134	LEU
1	F	139	VAL
1	F	142	LEU
1	F	166	HIS
1	F	180	ARG
1	F	184	THR
1	F	215	LEU
1	F	259	ARG
1	F	294	GLU
1	F	312	ARG
1	G	32	ASP
1	G	33	ASP
1	G	45	ASP
1	G	56	GLU
1	G	57	VAL
1	G	71	ARG
1	G	86	LEU
1	G	107	GLN
1	G	134	LEU
1	G	142	LEU
1	G	143	ILE
1	G	148	LYS
1	G	166	HIS
1	G	180	ARG
1	G	184	THR
1	G	215	LEU
1	G	294	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	302	LYS
1	H	33	ASP
1	H	56	GLU
1	H	57	VAL
1	H	86	LEU
1	H	107	GLN
1	H	134	LEU
1	H	142	LEU
1	H	166	HIS
1	H	175	SER
1	H	180	ARG
1	H	184	THR
1	H	215	LEU
1	H	294	GLU
1	H	302	LYS
1	H	303	ARG
1	I	21	ASP
1	I	44	ASP
1	I	56	GLU
1	I	57	VAL
1	I	71	ARG
1	I	86	LEU
1	I	95	LYS
1	I	107	GLN
1	I	134	LEU
1	I	142	LEU
1	I	166	HIS
1	I	175	SER
1	I	180	ARG
1	I	215	LEU
1	I	294	GLU
1	I	296	ARG
1	I	302	LYS
1	I	303	ARG
1	I	308	SER
1	J	23	LYS
1	J	43	VAL
1	J	44	ASP
1	J	56	GLU
1	J	58	ARG
1	J	67	ASP
1	J	86	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	107	GLN
1	J	134	LEU
1	J	142	LEU
1	J	166	HIS
1	J	215	LEU
1	J	224	MET
1	J	293	VAL
1	J	294	GLU
1	J	296	ARG
1	J	302	LYS
1	K	56	GLU
1	K	58	ARG
1	K	71	ARG
1	K	86	LEU
1	K	95	LYS
1	K	107	GLN
1	K	142	LEU
1	K	166	HIS
1	K	202	ARG
1	K	215	LEU
1	K	224	MET
1	K	294	GLU
1	K	302	LYS
1	K	308	SER
1	L	23	LYS
1	L	29	ASP
1	L	56	GLU
1	L	58	ARG
1	L	86	LEU
1	L	107	GLN
1	L	134	LEU
1	L	142	LEU
1	L	144	ARG
1	L	166	HIS
1	L	175	SER
1	L	215	LEU
1	L	294	GLU
1	L	302	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	HIS
1	B	135	HIS
1	B	236	HIS
1	C	107	GLN
1	C	236	HIS
1	C	301	GLN
1	D	135	HIS
1	D	225	HIS
1	D	236	HIS
1	E	107	GLN
1	E	225	HIS
1	E	236	HIS
1	F	107	GLN
1	F	135	HIS
1	F	236	HIS
1	F	256	GLN
1	G	107	GLN
1	G	135	HIS
1	G	236	HIS
1	H	135	HIS
1	H	225	HIS
1	H	236	HIS
1	H	301	GLN
1	I	135	HIS
1	I	203	GLN
1	I	236	HIS
1	J	236	HIS
1	K	236	HIS
1	L	135	HIS
1	L	236	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	CAA	G	507	-	53,56,56	1.34	9 (16%)	77,83,83	2.21	20 (25%)
2	CAA	F	506	-	53,56,56	1.30	8 (15%)	77,83,83	2.18	18 (23%)
2	CAA	C	503	-	53,56,56	1.22	6 (11%)	77,83,83	2.16	18 (23%)
2	CAA	K	500	-	53,56,56	1.30	9 (16%)	77,83,83	2.17	19 (24%)
2	CAA	B	502	-	53,56,56	1.23	8 (15%)	77,83,83	2.17	20 (25%)
2	CAA	H	508	-	53,56,56	1.35	9 (16%)	77,83,83	2.22	22 (28%)
2	CAA	E	505	-	53,56,56	1.26	6 (11%)	77,83,83	2.24	21 (27%)
2	CAA	J	510	-	53,56,56	1.27	7 (13%)	77,83,83	2.15	21 (27%)
2	CAA	D	504	-	53,56,56	1.28	8 (15%)	77,83,83	2.14	19 (24%)
2	CAA	I	509	-	53,56,56	1.37	8 (15%)	77,83,83	2.19	20 (25%)
2	CAA	A	501	-	53,56,56	1.28	7 (13%)	77,83,83	2.18	19 (24%)
2	CAA	L	511	-	53,56,56	1.20	8 (15%)	77,83,83	2.15	20 (25%)

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	CAA	G	507	-	-	14/55/71/71	0/3/3/3
2	CAA	F	506	-	-	16/55/71/71	0/3/3/3
2	CAA	C	503	-	-	12/55/71/71	0/3/3/3
2	CAA	K	500	-	-	16/55/71/71	0/3/3/3
2	CAA	B	502	-	-	11/55/71/71	0/3/3/3
2	CAA	H	508	-	-	14/55/71/71	0/3/3/3
2	CAA	E	505	-	-	13/55/71/71	0/3/3/3
2	CAA	J	510	-	-	15/55/71/71	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAA	D	504	-	-	15/55/71/71	0/3/3/3
2	CAA	I	509	-	-	17/55/71/71	0/3/3/3
2	CAA	A	501	-	-	13/55/71/71	0/3/3/3
2	CAA	L	511	-	-	14/55/71/71	0/3/3/3

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	506	CAA	C9P-N8P	4.16	1.43	1.33
2	E	505	CAA	C9P-N8P	4.02	1.43	1.33
2	K	500	CAA	C9P-N8P	3.99	1.43	1.33
2	H	508	CAA	C9P-N8P	3.88	1.42	1.33
2	D	504	CAA	C9P-N8P	3.87	1.42	1.33
2	H	508	CAA	P1A-O3A	-3.85	1.55	1.59
2	A	501	CAA	C9P-N8P	3.84	1.42	1.33
2	I	509	CAA	P1A-O3A	-3.80	1.55	1.59
2	G	507	CAA	C9P-N8P	3.77	1.42	1.33
2	C	503	CAA	C9P-N8P	3.77	1.42	1.33
2	I	509	CAA	C9P-N8P	3.76	1.42	1.33
2	L	511	CAA	C9P-N8P	3.72	1.42	1.33
2	J	510	CAA	C9P-N8P	3.60	1.42	1.33
2	F	506	CAA	P2A-O3A	-3.59	1.55	1.59
2	G	507	CAA	P3B-O3B	-3.56	1.53	1.59
2	B	502	CAA	C9P-N8P	3.51	1.41	1.33
2	D	504	CAA	P1A-O3A	-3.46	1.55	1.59
2	I	509	CAA	P3B-O3B	-3.23	1.53	1.59
2	I	509	CAA	P2A-O3A	-3.21	1.56	1.59
2	J	510	CAA	P3B-O3B	-3.20	1.53	1.59
2	A	501	CAA	P3B-O3B	-3.20	1.53	1.59
2	E	505	CAA	P3B-O3B	-3.14	1.54	1.59
2	C	503	CAA	P3B-O3B	-3.07	1.54	1.59
2	G	507	CAA	P2A-O3A	-3.01	1.56	1.59
2	H	508	CAA	P2A-O3A	-2.98	1.56	1.59
2	H	508	CAA	C5P-N4P	2.90	1.40	1.33
2	L	511	CAA	P3B-O3B	-2.85	1.54	1.59
2	H	508	CAA	P3B-O3B	-2.82	1.54	1.59
2	J	510	CAA	C5P-N4P	2.82	1.40	1.33
2	B	502	CAA	P3B-O3B	-2.82	1.54	1.59
2	K	500	CAA	P3B-O3B	-2.81	1.54	1.59
2	F	506	CAA	P1A-O3A	-2.79	1.56	1.59
2	A	501	CAA	C5P-N4P	2.78	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	504	CAA	P3B-O3B	-2.77	1.54	1.59
2	F	506	CAA	C5P-N4P	2.77	1.39	1.33
2	I	509	CAA	C5P-N4P	2.75	1.39	1.33
2	A	501	CAA	P1A-O3A	-2.73	1.56	1.59
2	B	502	CAA	C5P-N4P	2.68	1.39	1.33
2	B	502	CAA	C7P-N8P	-2.67	1.40	1.46
2	I	509	CAA	OAP-CAP	2.67	1.47	1.42
2	E	505	CAA	C5P-N4P	2.66	1.39	1.33
2	D	504	CAA	C5P-N4P	2.64	1.39	1.33
2	A	501	CAA	OAP-CAP	2.64	1.47	1.42
2	C	503	CAA	C5P-N4P	2.61	1.39	1.33
2	D	504	CAA	C7P-N8P	-2.61	1.40	1.46
2	G	507	CAA	C5P-N4P	2.59	1.39	1.33
2	K	500	CAA	C5P-N4P	2.59	1.39	1.33
2	L	511	CAA	C5P-N4P	2.59	1.39	1.33
2	G	507	CAA	C3P-N4P	-2.54	1.40	1.46
2	I	509	CAA	C3P-N4P	-2.52	1.40	1.46
2	F	506	CAA	C3P-N4P	-2.51	1.40	1.46
2	K	500	CAA	P2A-O3A	-2.49	1.56	1.59
2	H	508	CAA	C3P-N4P	-2.49	1.40	1.46
2	K	500	CAA	C3P-N4P	-2.47	1.40	1.46
2	F	506	CAA	P3B-O3B	-2.44	1.55	1.59
2	F	506	CAA	C7P-N8P	-2.41	1.40	1.46
2	D	504	CAA	C3P-N4P	-2.41	1.40	1.46
2	J	510	CAA	C3P-N4P	-2.41	1.40	1.46
2	K	500	CAA	OAP-CAP	2.41	1.46	1.42
2	A	501	CAA	C7P-N8P	-2.40	1.40	1.46
2	A	501	CAA	C3P-N4P	-2.39	1.40	1.46
2	C	503	CAA	C3P-N4P	-2.38	1.40	1.46
2	K	500	CAA	C7P-N8P	-2.36	1.40	1.46
2	K	500	CAA	P1A-O3A	-2.36	1.57	1.59
2	E	505	CAA	C3P-N4P	-2.35	1.40	1.46
2	B	502	CAA	C3P-N4P	-2.35	1.40	1.46
2	C	503	CAA	C7P-N8P	-2.35	1.40	1.46
2	J	510	CAA	P2A-O3A	-2.35	1.57	1.59
2	L	511	CAA	C3P-N4P	-2.35	1.40	1.46
2	G	507	CAA	P1A-O3A	-2.34	1.57	1.59
2	E	505	CAA	C7P-N8P	-2.33	1.40	1.46
2	C	503	CAA	P1A-O3A	-2.29	1.57	1.59
2	L	511	CAA	P1A-O3A	-2.27	1.57	1.59
2	J	510	CAA	C7P-N8P	-2.26	1.41	1.46
2	G	507	CAA	C7P-N8P	-2.25	1.41	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	508	CAA	OAP-CAP	2.22	1.46	1.42
2	I	509	CAA	C7P-N8P	-2.21	1.41	1.46
2	B	502	CAA	OAP-CAP	2.21	1.46	1.42
2	D	504	CAA	OAP-CAP	2.20	1.46	1.42
2	H	508	CAA	C7P-N8P	-2.20	1.41	1.46
2	J	510	CAA	P1A-O3A	-2.15	1.57	1.59
2	B	502	CAA	P1A-O3A	-2.11	1.57	1.59
2	G	507	CAA	P1A-O5B	-2.10	1.51	1.59
2	L	511	CAA	C7P-N8P	-2.09	1.41	1.46
2	L	511	CAA	P1A-O5B	-2.07	1.51	1.59
2	D	504	CAA	P1A-O5B	-2.07	1.51	1.59
2	H	508	CAA	P1A-O5B	-2.07	1.51	1.59
2	G	507	CAA	OAP-CAP	2.06	1.46	1.42
2	L	511	CAA	OAP-CAP	2.05	1.45	1.42
2	B	502	CAA	P2A-O3A	-2.03	1.57	1.59
2	E	505	CAA	P2A-O3A	-2.03	1.57	1.59
2	F	506	CAA	OAP-CAP	2.02	1.45	1.42
2	K	500	CAA	P1A-O5B	-2.01	1.51	1.59

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	505	CAA	N9A-C8A-N7A	-7.93	102.69	113.94
2	L	511	CAA	N9A-C8A-N7A	-7.77	102.92	113.94
2	H	508	CAA	N9A-C8A-N7A	-7.76	102.93	113.94
2	A	501	CAA	N9A-C8A-N7A	-7.72	102.99	113.94
2	G	507	CAA	N9A-C8A-N7A	-7.69	103.02	113.94
2	K	500	CAA	N9A-C8A-N7A	-7.60	103.15	113.94
2	F	506	CAA	N9A-C8A-N7A	-7.57	103.19	113.94
2	E	505	CAA	C4A-N9A-C8A	7.52	113.64	105.74
2	B	502	CAA	N9A-C8A-N7A	-7.44	103.38	113.94
2	I	509	CAA	N9A-C8A-N7A	-7.43	103.39	113.94
2	K	500	CAA	C4A-N9A-C8A	7.39	113.50	105.74
2	J	510	CAA	N9A-C8A-N7A	-7.35	103.51	113.94
2	C	503	CAA	N9A-C8A-N7A	-7.34	103.52	113.94
2	D	504	CAA	N9A-C8A-N7A	-7.33	103.53	113.94
2	H	508	CAA	C4A-N9A-C8A	7.33	113.43	105.74
2	L	511	CAA	C4A-N9A-C8A	7.31	113.42	105.74
2	B	502	CAA	C4A-N9A-C8A	7.23	113.33	105.74
2	G	507	CAA	C4A-N9A-C8A	7.16	113.25	105.74
2	D	504	CAA	C4A-N9A-C8A	7.15	113.25	105.74
2	A	501	CAA	C4A-N9A-C8A	7.12	113.22	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	506	CAA	C4A-N9A-C8A	7.03	113.12	105.74
2	C	503	CAA	C4A-N9A-C8A	6.89	112.97	105.74
2	J	510	CAA	C4A-N9A-C8A	6.81	112.88	105.74
2	I	509	CAA	C4A-N9A-C8A	6.64	112.71	105.74
2	C	503	CAA	O4B-C1B-N9A	6.21	120.01	108.09
2	E	505	CAA	C5A-N7A-C8A	6.00	112.88	103.45
2	H	508	CAA	C5A-N7A-C8A	5.96	112.82	103.45
2	G	507	CAA	O4B-C1B-N9A	5.94	119.49	108.09
2	A	501	CAA	O4B-C1B-N9A	5.94	119.49	108.09
2	E	505	CAA	O4B-C1B-N9A	5.93	119.47	108.09
2	B	502	CAA	O4B-C1B-N9A	5.92	119.47	108.09
2	G	507	CAA	C5A-N7A-C8A	5.86	112.66	103.45
2	L	511	CAA	O4B-C1B-N9A	5.85	119.32	108.09
2	F	506	CAA	O4B-C1B-N9A	5.80	119.23	108.09
2	I	509	CAA	C5A-N7A-C8A	5.79	112.55	103.45
2	K	500	CAA	O4B-C1B-N9A	5.79	119.20	108.09
2	F	506	CAA	C5A-N7A-C8A	5.74	112.47	103.45
2	J	510	CAA	O4B-C1B-N9A	5.73	119.09	108.09
2	I	509	CAA	O4B-C1B-N9A	5.71	119.05	108.09
2	A	501	CAA	C5A-N7A-C8A	5.70	112.41	103.45
2	H	508	CAA	O4B-C1B-N9A	5.65	118.94	108.09
2	D	504	CAA	O4B-C1B-N9A	5.64	118.93	108.09
2	K	500	CAA	C5A-N7A-C8A	5.63	112.29	103.45
2	C	503	CAA	C5A-N7A-C8A	5.57	112.20	103.45
2	L	511	CAA	C5A-N7A-C8A	5.56	112.19	103.45
2	B	502	CAA	C5A-N7A-C8A	5.55	112.17	103.45
2	J	510	CAA	C5A-N7A-C8A	5.55	112.17	103.45
2	D	504	CAA	C5A-N7A-C8A	5.28	111.75	103.45
2	F	506	CAA	C2-C1-S1P	4.37	119.17	113.63
2	I	509	CAA	C2P-S1P-C1	4.10	113.97	101.84
2	K	500	CAA	C2P-S1P-C1	4.06	113.83	101.84
2	A	501	CAA	C2P-S1P-C1	3.98	113.60	101.84
2	H	508	CAA	C2P-S1P-C1	3.96	113.56	101.84
2	C	503	CAA	C2P-S1P-C1	3.94	113.48	101.84
2	H	508	CAA	O3B-C3B-C2B	-3.93	97.58	111.68
2	G	507	CAA	C2P-S1P-C1	3.92	113.42	101.84
2	A	501	CAA	O3B-C3B-C2B	-3.89	97.71	111.68
2	G	507	CAA	O3B-C3B-C4B	-3.88	96.35	110.03
2	F	506	CAA	C2P-S1P-C1	3.88	113.30	101.84
2	L	511	CAA	C2P-S1P-C1	3.86	113.26	101.84
2	D	504	CAA	C2P-S1P-C1	3.81	113.11	101.84
2	E	505	CAA	C2P-S1P-C1	3.78	113.02	101.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	510	CAA	C2P-S1P-C1	3.77	112.98	101.84
2	I	509	CAA	O3B-C3B-C2B	-3.76	98.20	111.68
2	I	509	CAA	C2-C1-S1P	3.72	118.35	113.63
2	B	502	CAA	C2P-S1P-C1	3.71	112.81	101.84
2	E	505	CAA	C2-C1-S1P	3.69	118.31	113.63
2	E	505	CAA	O3B-C3B-C2B	-3.67	98.50	111.68
2	D	504	CAA	O3B-C3B-C2B	-3.67	98.51	111.68
2	B	502	CAA	O3B-C3B-C2B	-3.67	98.52	111.68
2	F	506	CAA	C3B-C2B-C1B	3.64	107.89	99.89
2	F	506	CAA	O3B-C3B-C2B	-3.63	98.66	111.68
2	I	509	CAA	O1-C1-S1P	-3.63	118.07	122.68
2	H	508	CAA	C2-C1-S1P	3.63	118.24	113.63
2	L	511	CAA	C3B-C2B-C1B	3.63	107.86	99.89
2	G	507	CAA	O3B-C3B-C2B	-3.62	98.69	111.68
2	I	509	CAA	C3B-C2B-C1B	3.61	107.82	99.89
2	A	501	CAA	O3-C3-C4	-3.60	112.45	121.48
2	K	500	CAA	C2-C1-S1P	3.59	118.19	113.63
2	C	503	CAA	O3B-C3B-C4B	-3.57	97.44	110.03
2	I	509	CAA	O3B-C3B-C4B	-3.57	97.45	110.03
2	C	503	CAA	C2-C1-S1P	3.56	118.15	113.63
2	J	510	CAA	C2-C1-S1P	3.56	118.15	113.63
2	E	505	CAA	O3B-C3B-C4B	-3.56	97.48	110.03
2	C	503	CAA	O3B-C3B-C2B	-3.55	98.93	111.68
2	D	504	CAA	O3B-C3B-C4B	-3.55	97.52	110.03
2	H	508	CAA	C3B-C2B-C1B	3.52	107.63	99.89
2	E	505	CAA	C3B-C2B-C1B	3.52	107.63	99.89
2	K	500	CAA	O3B-C3B-C4B	-3.51	97.67	110.03
2	H	508	CAA	O3B-C3B-C4B	-3.50	97.67	110.03
2	C	503	CAA	O3-C3-C4	-3.50	112.71	121.48
2	D	504	CAA	C2-C1-S1P	3.50	118.07	113.63
2	D	504	CAA	C3B-C2B-C1B	3.50	107.58	99.89
2	G	507	CAA	C2-C1-S1P	3.49	118.06	113.63
2	I	509	CAA	O3-C3-C4	-3.48	112.77	121.48
2	L	511	CAA	O3B-C3B-C4B	-3.46	97.83	110.03
2	J	510	CAA	C3B-C2B-C1B	3.45	107.49	99.89
2	L	511	CAA	O3B-C3B-C2B	-3.44	99.33	111.68
2	B	502	CAA	C3B-C2B-C1B	3.44	107.45	99.89
2	J	510	CAA	O3B-C3B-C2B	-3.44	99.35	111.68
2	B	502	CAA	O3-C3-C4	-3.42	112.91	121.48
2	G	507	CAA	C3B-C2B-C1B	3.42	107.41	99.89
2	I	509	CAA	C4B-O4B-C1B	3.42	117.02	109.47
2	K	500	CAA	C3B-C2B-C1B	3.41	107.39	99.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	500	CAA	O3-C3-C4	-3.41	112.94	121.48
2	A	501	CAA	C3B-C2B-C1B	3.41	107.38	99.89
2	L	511	CAA	O3-C3-C4	-3.40	112.97	121.48
2	G	507	CAA	O3-C3-C4	-3.39	112.99	121.48
2	E	505	CAA	O3-C3-C4	-3.38	113.01	121.48
2	D	504	CAA	O3-C3-C4	-3.36	113.07	121.48
2	G	507	CAA	C4B-O4B-C1B	3.35	116.87	109.47
2	B	502	CAA	C2-C1-S1P	3.35	117.89	113.63
2	J	510	CAA	O3-C3-C4	-3.33	113.14	121.48
2	C	503	CAA	C3B-C2B-C1B	3.33	107.21	99.89
2	K	500	CAA	O3B-C3B-C2B	-3.32	99.75	111.68
2	A	501	CAA	C2-C1-S1P	3.29	117.81	113.63
2	H	508	CAA	C4B-O4B-C1B	3.28	116.72	109.47
2	F	506	CAA	O3-C3-C4	-3.28	113.27	121.48
2	C	503	CAA	O1-C1-S1P	-3.28	118.51	122.68
2	A	501	CAA	C4B-O4B-C1B	3.26	116.67	109.47
2	J	510	CAA	C4B-O4B-C1B	3.25	116.64	109.47
2	J	510	CAA	O1-C1-S1P	-3.19	118.62	122.68
2	B	502	CAA	O3B-C3B-C4B	-3.19	98.79	110.03
2	J	510	CAA	O3B-C3B-C4B	-3.19	98.79	110.03
2	H	508	CAA	O3-C3-C4	-3.18	113.53	121.48
2	F	506	CAA	O3B-C3B-C4B	-3.15	98.93	110.03
2	D	504	CAA	O1-C1-S1P	-3.15	118.68	122.68
2	A	501	CAA	O1-C1-S1P	-3.14	118.69	122.68
2	F	506	CAA	O1-C1-S1P	-3.13	118.70	122.68
2	A	501	CAA	O3B-C3B-C4B	-3.12	99.04	110.03
2	K	500	CAA	O1-C1-S1P	-3.10	118.74	122.68
2	J	510	CAA	C3-C2-C1	3.10	126.09	113.95
2	L	511	CAA	C2-C1-S1P	3.09	117.55	113.63
2	H	508	CAA	C4A-C5A-N7A	-3.07	107.08	110.58
2	B	502	CAA	C3-C2-C1	3.04	125.87	113.95
2	I	509	CAA	C3-C2-C1	3.01	125.78	113.95
2	C	503	CAA	C3-C2-C1	3.01	125.77	113.95
2	A	501	CAA	C3-C2-C1	3.00	125.70	113.95
2	F	506	CAA	C4B-O4B-C1B	2.98	116.05	109.47
2	B	502	CAA	C4B-O4B-C1B	2.97	116.03	109.47
2	B	502	CAA	O1-C1-S1P	-2.97	118.91	122.68
2	L	511	CAA	C3-C2-C1	2.95	125.51	113.95
2	E	505	CAA	C3-C2-C1	2.94	125.50	113.95
2	F	506	CAA	C3-C2-C1	2.93	125.45	113.95
2	D	504	CAA	C3-C2-C1	2.93	125.45	113.95
2	H	508	CAA	C3-C2-C1	2.92	125.40	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	507	CAA	C3-C2-C1	2.89	125.30	113.95
2	E	505	CAA	C4A-C5A-N7A	-2.89	107.28	110.58
2	C	503	CAA	C4B-O4B-C1B	2.87	115.80	109.47
2	K	500	CAA	C3-C2-C1	2.85	125.11	113.95
2	L	511	CAA	C4B-O4B-C1B	2.84	115.73	109.47
2	H	508	CAA	O1-C1-S1P	-2.80	119.12	122.68
2	E	505	CAA	C4B-O4B-C1B	2.80	115.64	109.47
2	F	506	CAA	C4A-C5A-N7A	-2.79	107.39	110.58
2	E	505	CAA	O1-C1-S1P	-2.79	119.13	122.68
2	K	500	CAA	N3A-C4A-N9A	2.78	131.89	127.17
2	K	500	CAA	C4B-O4B-C1B	2.74	115.52	109.47
2	C	503	CAA	N3A-C4A-N9A	2.74	131.83	127.17
2	D	504	CAA	C4B-O4B-C1B	2.72	115.47	109.47
2	G	507	CAA	C4A-C5A-N7A	-2.70	107.50	110.58
2	I	509	CAA	C4A-C5A-N7A	-2.69	107.50	110.58
2	E	505	CAA	N3A-C4A-N9A	2.69	131.74	127.17
2	B	502	CAA	N3A-C4A-N9A	2.68	131.73	127.17
2	C	503	CAA	C4A-C5A-N7A	-2.66	107.53	110.58
2	K	500	CAA	C4A-C5A-N7A	-2.66	107.54	110.58
2	A	501	CAA	N3A-C4A-N9A	2.66	131.68	127.17
2	J	510	CAA	C4A-C5A-N7A	-2.60	107.61	110.58
2	L	511	CAA	N3A-C4A-N9A	2.57	131.54	127.17
2	B	502	CAA	C4A-C5A-N7A	-2.57	107.64	110.58
2	G	507	CAA	C5B-C4B-C3B	-2.55	105.89	114.38
2	L	511	CAA	O1-C1-S1P	-2.54	119.45	122.68
2	E	505	CAA	C5B-C4B-C3B	-2.53	105.96	114.38
2	I	509	CAA	N3A-C4A-N9A	2.52	131.46	127.17
2	D	504	CAA	N3A-C4A-N9A	2.49	131.41	127.17
2	A	501	CAA	C4A-C5A-N7A	-2.49	107.73	110.58
2	H	508	CAA	C4A-N9A-C1B	-2.48	120.83	126.63
2	J	510	CAA	N3A-C4A-N9A	2.46	131.35	127.17
2	H	508	CAA	N3A-C4A-N9A	2.43	131.30	127.17
2	D	504	CAA	C5B-C4B-C3B	-2.43	106.29	114.38
2	F	506	CAA	N3A-C4A-N9A	2.41	131.27	127.17
2	G	507	CAA	O1-C1-S1P	-2.37	119.67	122.68
2	G	507	CAA	C4A-N9A-C1B	-2.36	121.11	126.63
2	I	509	CAA	C5B-C4B-C3B	-2.36	106.51	114.38
2	G	507	CAA	N3A-C4A-N9A	2.36	131.18	127.17
2	C	503	CAA	C5B-C4B-C3B	-2.35	106.54	114.38
2	A	501	CAA	C4-C3-C2	2.34	125.87	117.78
2	L	511	CAA	C4A-C5A-N7A	-2.30	107.95	110.58
2	J	510	CAA	C4A-N9A-C1B	-2.30	121.26	126.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	CAA	C4-C3-C2	2.29	125.69	117.78
2	K	500	CAA	C4A-N9A-C1B	-2.28	121.30	126.63
2	D	504	CAA	C4A-N9A-C1B	-2.28	121.31	126.63
2	A	501	CAA	C5B-C4B-C3B	-2.27	106.82	114.38
2	D	504	CAA	C4A-C5A-N7A	-2.27	107.99	110.58
2	G	507	CAA	C4-C3-C2	2.25	125.58	117.78
2	E	505	CAA	C4A-N9A-C1B	-2.25	121.38	126.63
2	I	509	CAA	O2A-P1A-O3A	2.24	113.34	107.27
2	J	510	CAA	O5P-C5P-C6P	-2.24	117.95	122.02
2	F	506	CAA	O2A-P1A-O3A	2.22	113.27	107.27
2	H	508	CAA	P3B-O3B-C3B	2.21	129.32	123.43
2	L	511	CAA	C5B-C4B-C3B	-2.20	107.06	114.38
2	D	504	CAA	C4-C3-C2	2.19	125.34	117.78
2	B	502	CAA	C5B-C4B-C3B	-2.18	107.12	114.38
2	L	511	CAA	C4A-N9A-C1B	-2.17	121.55	126.63
2	E	505	CAA	O2A-P1A-O3A	2.17	113.13	107.27
2	G	507	CAA	O2A-P1A-O3A	2.17	113.13	107.27
2	C	503	CAA	C4A-N9A-C1B	-2.15	121.60	126.63
2	J	510	CAA	C4-C3-C2	2.15	125.22	117.78
2	B	502	CAA	C5A-C4A-N9A	-2.15	103.47	105.81
2	F	506	CAA	C5B-C4B-C3B	-2.14	107.24	114.38
2	D	504	CAA	C5A-C4A-N9A	-2.14	103.48	105.81
2	A	501	CAA	C4A-N9A-C1B	-2.14	121.63	126.63
2	I	509	CAA	C4-C3-C2	2.14	125.17	117.78
2	J	510	CAA	O2B-C2B-C1B	2.13	117.44	110.10
2	L	511	CAA	C4-C3-C2	2.12	125.13	117.78
2	J	510	CAA	P3B-O3B-C3B	2.12	129.10	123.43
2	I	509	CAA	C4A-N9A-C1B	-2.11	121.69	126.63
2	F	506	CAA	C4A-N9A-C1B	-2.11	121.70	126.63
2	E	505	CAA	C5A-C4A-N9A	-2.11	103.51	105.81
2	E	505	CAA	C4-C3-C2	2.11	125.08	117.78
2	K	500	CAA	C5A-C4A-N9A	-2.10	103.52	105.81
2	H	508	CAA	C5B-C4B-C3B	-2.10	107.37	114.38
2	L	511	CAA	C5A-C4A-N9A	-2.10	103.53	105.81
2	B	502	CAA	C4A-N9A-C1B	-2.09	121.74	126.63
2	K	500	CAA	C4-C3-C2	2.08	124.99	117.78
2	A	501	CAA	O2B-C2B-C1B	2.06	117.19	110.10
2	G	507	CAA	C5A-C4A-N9A	-2.05	103.57	105.81
2	H	508	CAA	O2B-C2B-C1B	2.05	117.17	110.10
2	H	508	CAA	C4-C3-C2	2.05	124.86	117.78
2	E	505	CAA	O2B-C2B-C1B	2.04	117.14	110.10
2	B	502	CAA	C4-C3-C2	2.04	124.82	117.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	508	CAA	C6A-C5A-N7A	2.03	136.01	132.09
2	K	500	CAA	P3B-O3B-C3B	2.03	128.86	123.43
2	J	510	CAA	O2A-P1A-O3A	2.02	112.74	107.27
2	L	511	CAA	P3B-O3B-C3B	2.01	128.80	123.43
2	H	508	CAA	O2A-P1A-O3A	2.01	112.71	107.27
2	I	509	CAA	O2B-C2B-C1B	2.01	117.02	110.10
2	B	502	CAA	O2B-C2B-C1B	2.00	117.01	110.10

There are no chirality outliers.

All (170) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CAA	CAP-C9P-N8P-C7P
2	A	501	CAA	C6P-C5P-N4P-C3P
2	A	501	CAA	O5P-C5P-N4P-C3P
2	A	501	CAA	C1-C2-C3-C4
2	B	502	CAA	C6P-C5P-N4P-C3P
2	B	502	CAA	O5P-C5P-N4P-C3P
2	B	502	CAA	C1-C2-C3-C4
2	C	503	CAA	CAP-C9P-N8P-C7P
2	C	503	CAA	C6P-C5P-N4P-C3P
2	C	503	CAA	O5P-C5P-N4P-C3P
2	C	503	CAA	C1-C2-C3-C4
2	D	504	CAA	CAP-C9P-N8P-C7P
2	D	504	CAA	C6P-C5P-N4P-C3P
2	D	504	CAA	O5P-C5P-N4P-C3P
2	D	504	CAA	C1-C2-C3-C4
2	E	505	CAA	CAP-C9P-N8P-C7P
2	E	505	CAA	C6P-C5P-N4P-C3P
2	E	505	CAA	O5P-C5P-N4P-C3P
2	E	505	CAA	C1-C2-C3-C4
2	F	506	CAA	CAP-CBP-CCP-O6A
2	F	506	CAA	CAP-C9P-N8P-C7P
2	F	506	CAA	C6P-C5P-N4P-C3P
2	F	506	CAA	O5P-C5P-N4P-C3P
2	F	506	CAA	C1-C2-C3-C4
2	G	507	CAA	CDP-CBP-CCP-O6A
2	G	507	CAA	CEP-CBP-CCP-O6A
2	G	507	CAA	CAP-CBP-CCP-O6A
2	G	507	CAA	CAP-C9P-N8P-C7P
2	G	507	CAA	C6P-C5P-N4P-C3P
2	G	507	CAA	O5P-C5P-N4P-C3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	507	CAA	C1-C2-C3-C4
2	H	508	CAA	CAP-C9P-N8P-C7P
2	H	508	CAA	C6P-C5P-N4P-C3P
2	H	508	CAA	O5P-C5P-N4P-C3P
2	H	508	CAA	C1-C2-C3-C4
2	I	509	CAA	CAP-C9P-N8P-C7P
2	I	509	CAA	C6P-C5P-N4P-C3P
2	I	509	CAA	O5P-C5P-N4P-C3P
2	I	509	CAA	C1-C2-C3-C4
2	J	510	CAA	CAP-C9P-N8P-C7P
2	J	510	CAA	C6P-C5P-N4P-C3P
2	J	510	CAA	O5P-C5P-N4P-C3P
2	J	510	CAA	C1-C2-C3-C4
2	K	500	CAA	CAP-CBP-CCP-O6A
2	K	500	CAA	CAP-C9P-N8P-C7P
2	K	500	CAA	C6P-C5P-N4P-C3P
2	K	500	CAA	O5P-C5P-N4P-C3P
2	K	500	CAA	C1-C2-C3-C4
2	L	511	CAA	CAP-C9P-N8P-C7P
2	L	511	CAA	C6P-C5P-N4P-C3P
2	L	511	CAA	O5P-C5P-N4P-C3P
2	L	511	CAA	C1-C2-C3-C4
2	J	510	CAA	C6P-C7P-N8P-C9P
2	B	502	CAA	C6P-C7P-N8P-C9P
2	H	508	CAA	C6P-C7P-N8P-C9P
2	I	509	CAA	C6P-C7P-N8P-C9P
2	K	500	CAA	C6P-C7P-N8P-C9P
2	C	503	CAA	C6P-C7P-N8P-C9P
2	G	507	CAA	C6P-C7P-N8P-C9P
2	L	511	CAA	C6P-C7P-N8P-C9P
2	A	501	CAA	C6P-C7P-N8P-C9P
2	D	504	CAA	C6P-C7P-N8P-C9P
2	F	506	CAA	C6P-C7P-N8P-C9P
2	E	505	CAA	C6P-C7P-N8P-C9P
2	D	504	CAA	O9P-C9P-N8P-C7P
2	F	506	CAA	O9P-C9P-N8P-C7P
2	A	501	CAA	O9P-C9P-N8P-C7P
2	E	505	CAA	O9P-C9P-N8P-C7P
2	G	507	CAA	O9P-C9P-N8P-C7P
2	L	511	CAA	O9P-C9P-N8P-C7P
2	C	503	CAA	O9P-C9P-N8P-C7P
2	J	510	CAA	O9P-C9P-N8P-C7P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	I	509	CAA	O9P-C9P-N8P-C7P
2	K	500	CAA	O9P-C9P-N8P-C7P
2	B	502	CAA	CAP-C9P-N8P-C7P
2	A	501	CAA	C1-C2-C3-O3
2	B	502	CAA	C1-C2-C3-O3
2	C	503	CAA	C1-C2-C3-O3
2	D	504	CAA	C1-C2-C3-O3
2	E	505	CAA	C1-C2-C3-O3
2	F	506	CAA	C1-C2-C3-O3
2	G	507	CAA	C1-C2-C3-O3
2	H	508	CAA	C1-C2-C3-O3
2	I	509	CAA	C1-C2-C3-O3
2	J	510	CAA	C1-C2-C3-O3
2	K	500	CAA	C1-C2-C3-O3
2	L	511	CAA	C1-C2-C3-O3
2	B	502	CAA	O9P-C9P-N8P-C7P
2	H	508	CAA	O9P-C9P-N8P-C7P
2	F	506	CAA	P1A-O3A-P2A-O6A
2	H	508	CAA	P1A-O3A-P2A-O6A
2	I	509	CAA	P1A-O3A-P2A-O6A
2	A	501	CAA	CDP-CBP-CCP-O6A
2	A	501	CAA	CEP-CBP-CCP-O6A
2	B	502	CAA	CDP-CBP-CCP-O6A
2	B	502	CAA	CEP-CBP-CCP-O6A
2	C	503	CAA	CDP-CBP-CCP-O6A
2	D	504	CAA	CDP-CBP-CCP-O6A
2	E	505	CAA	CDP-CBP-CCP-O6A
2	E	505	CAA	CEP-CBP-CCP-O6A
2	F	506	CAA	CDP-CBP-CCP-O6A
2	F	506	CAA	CEP-CBP-CCP-O6A
2	H	508	CAA	CDP-CBP-CCP-O6A
2	I	509	CAA	CDP-CBP-CCP-O6A
2	I	509	CAA	CEP-CBP-CCP-O6A
2	J	510	CAA	CDP-CBP-CCP-O6A
2	J	510	CAA	CEP-CBP-CCP-O6A
2	K	500	CAA	CDP-CBP-CCP-O6A
2	K	500	CAA	CEP-CBP-CCP-O6A
2	L	511	CAA	CDP-CBP-CCP-O6A
2	A	501	CAA	CAP-CBP-CCP-O6A
2	B	502	CAA	CAP-CBP-CCP-O6A
2	C	503	CAA	CAP-CBP-CCP-O6A
2	D	504	CAA	CAP-CBP-CCP-O6A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	505	CAA	CAP-CBP-CCP-O6A
2	H	508	CAA	CAP-CBP-CCP-O6A
2	I	509	CAA	CAP-CBP-CCP-O6A
2	J	510	CAA	CAP-CBP-CCP-O6A
2	L	511	CAA	CAP-CBP-CCP-O6A
2	A	501	CAA	CCP-O6A-P2A-O5A
2	D	504	CAA	CCP-O6A-P2A-O5A
2	E	505	CAA	CCP-O6A-P2A-O5A
2	F	506	CAA	CCP-O6A-P2A-O3A
2	F	506	CAA	CCP-O6A-P2A-O5A
2	G	507	CAA	CCP-O6A-P2A-O3A
2	G	507	CAA	CCP-O6A-P2A-O5A
2	I	509	CAA	CCP-O6A-P2A-O3A
2	I	509	CAA	CCP-O6A-P2A-O5A
2	J	510	CAA	CCP-O6A-P2A-O5A
2	K	500	CAA	CCP-O6A-P2A-O3A
2	K	500	CAA	CCP-O6A-P2A-O5A
2	L	511	CAA	CCP-O6A-P2A-O5A
2	A	501	CAA	C3B-O3B-P3B-O7A
2	B	502	CAA	C3B-O3B-P3B-O7A
2	C	503	CAA	C3B-O3B-P3B-O7A
2	D	504	CAA	C3B-O3B-P3B-O7A
2	E	505	CAA	C3B-O3B-P3B-O7A
2	F	506	CAA	C3B-O3B-P3B-O7A
2	G	507	CAA	C3B-O3B-P3B-O7A
2	H	508	CAA	C3B-O3B-P3B-O7A
2	I	509	CAA	C3B-O3B-P3B-O7A
2	J	510	CAA	C3B-O3B-P3B-O7A
2	K	500	CAA	C3B-O3B-P3B-O7A
2	L	511	CAA	C3B-O3B-P3B-O7A
2	D	504	CAA	P1A-O3A-P2A-O6A
2	J	510	CAA	P1A-O3A-P2A-O6A
2	A	501	CAA	O1-C1-C2-C3
2	C	503	CAA	O1-C1-C2-C3
2	E	505	CAA	O1-C1-C2-C3
2	F	506	CAA	O1-C1-C2-C3
2	J	510	CAA	O1-C1-C2-C3
2	L	511	CAA	O1-C1-C2-C3
2	D	504	CAA	P2A-O3A-P1A-O2A
2	F	506	CAA	P2A-O3A-P1A-O2A
2	I	509	CAA	P2A-O3A-P1A-O2A
2	J	510	CAA	P2A-O3A-P1A-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	K	500	CAA	P2A-O3A-P1A-O2A
2	I	509	CAA	C3B-O3B-P3B-O8A
2	K	500	CAA	C3B-O3B-P3B-O8A
2	C	503	CAA	CEP-CBP-CCP-O6A
2	D	504	CAA	CEP-CBP-CCP-O6A
2	H	508	CAA	CEP-CBP-CCP-O6A
2	L	511	CAA	CEP-CBP-CCP-O6A
2	D	504	CAA	O1-C1-C2-C3
2	G	507	CAA	O1-C1-C2-C3
2	H	508	CAA	O1-C1-C2-C3
2	I	509	CAA	O1-C1-C2-C3
2	K	500	CAA	O1-C1-C2-C3
2	H	508	CAA	P2A-O3A-P1A-O2A
2	L	511	CAA	P2A-O3A-P1A-O2A

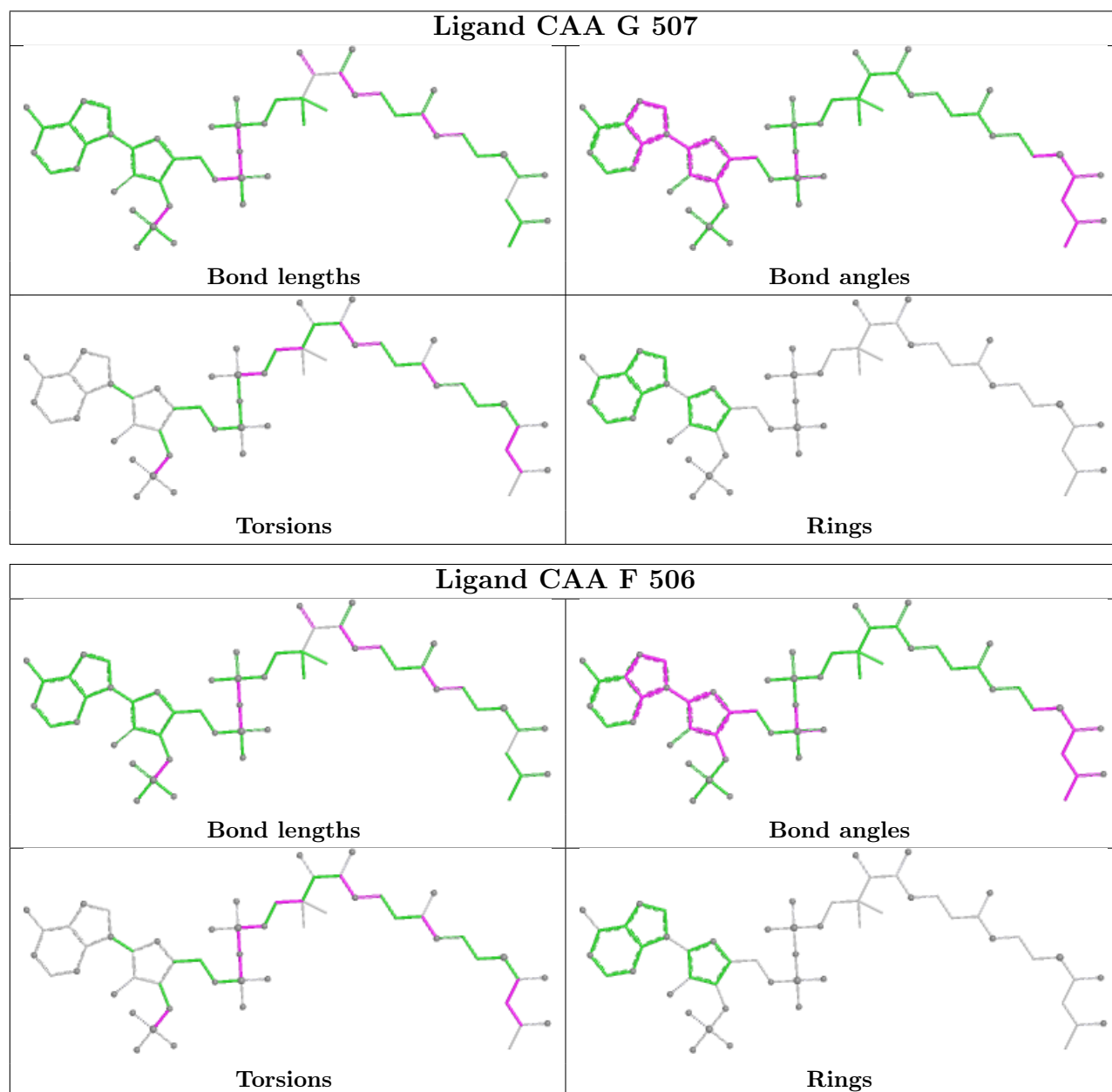
There are no ring outliers.

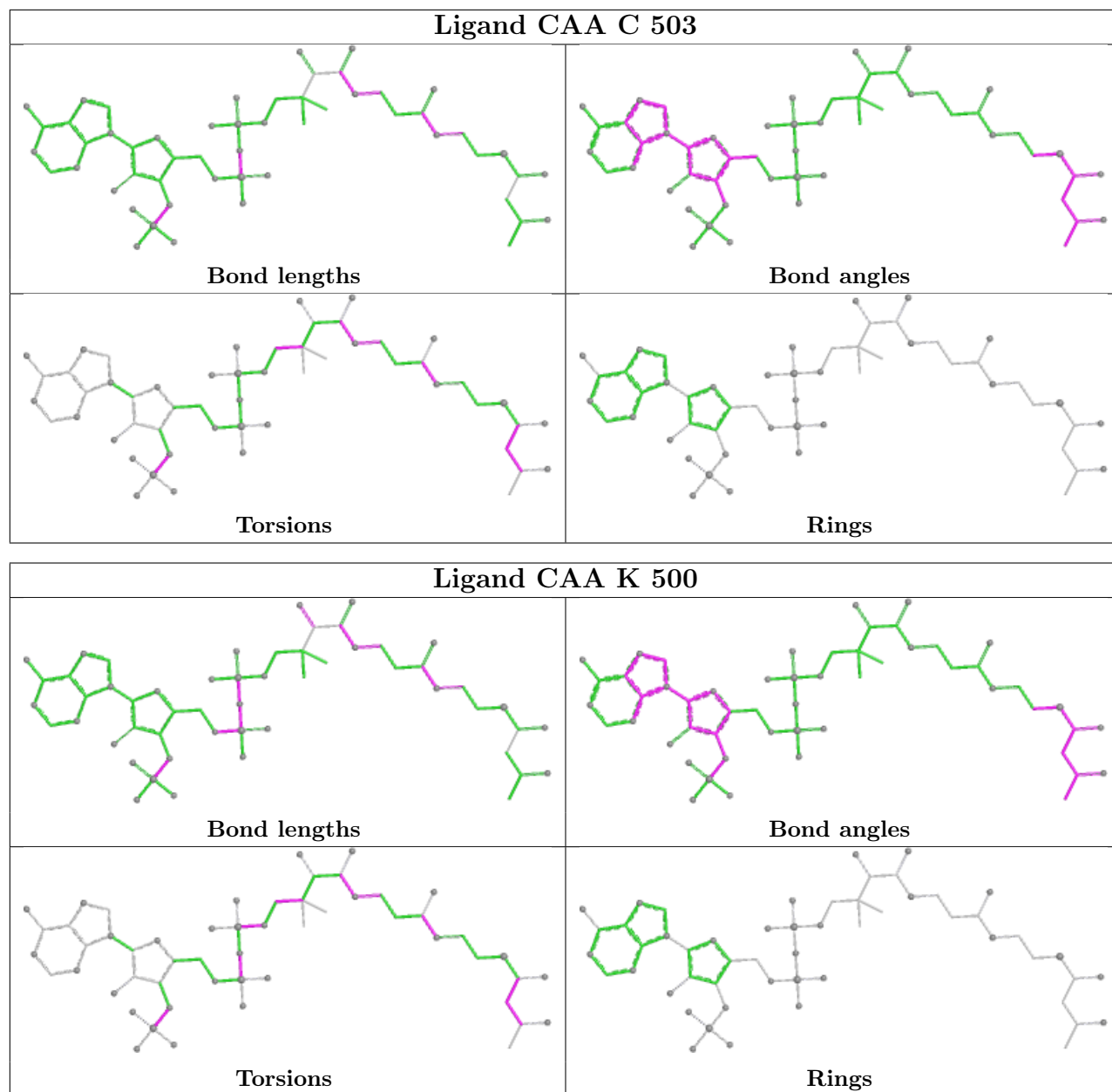
12 monomers are involved in 39 short contacts:

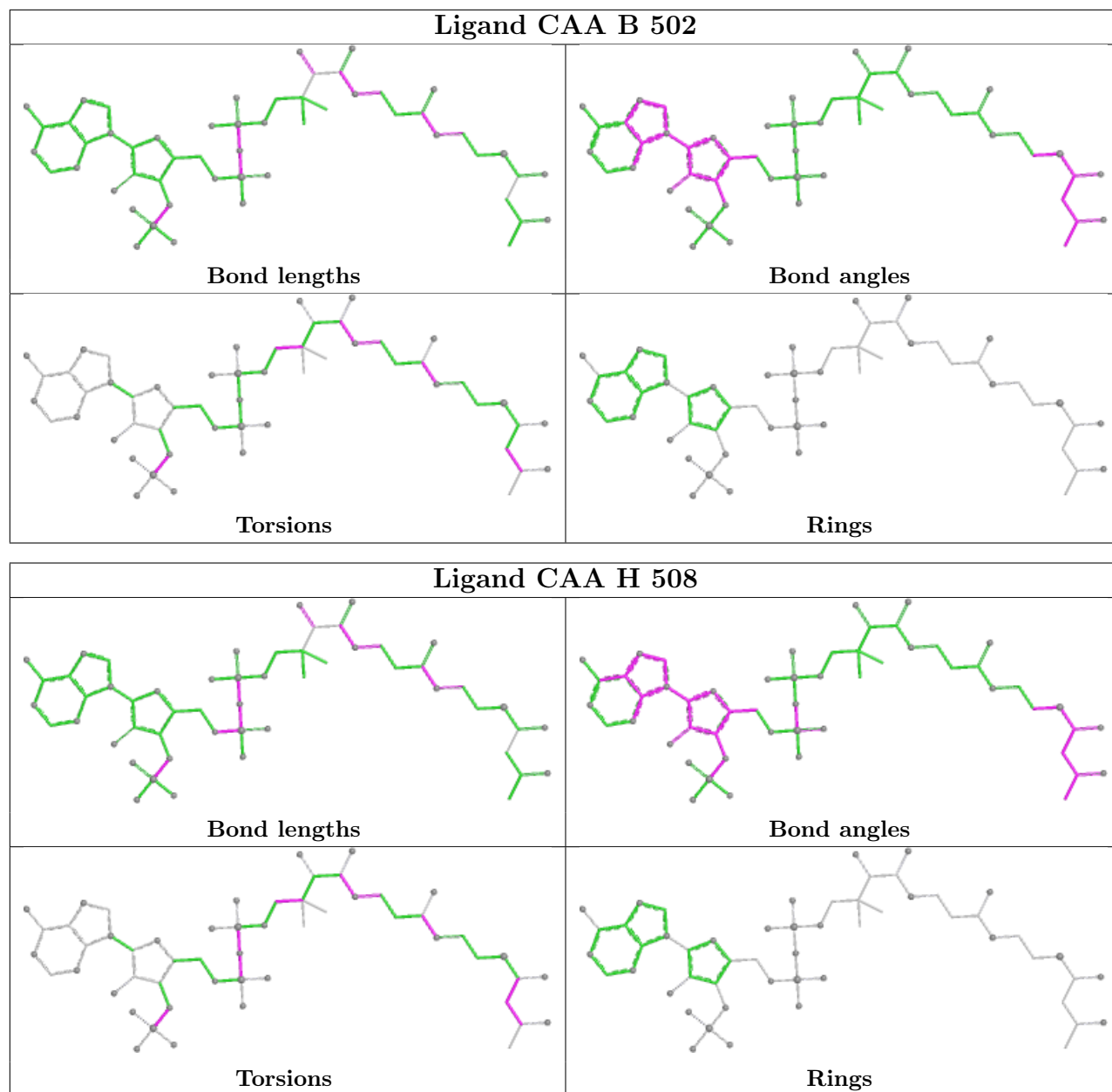
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	507	CAA	4	0
2	F	506	CAA	3	0
2	C	503	CAA	9	0
2	K	500	CAA	8	0
2	B	502	CAA	2	0
2	H	508	CAA	3	0
2	E	505	CAA	1	0
2	J	510	CAA	1	0
2	D	504	CAA	3	0
2	I	509	CAA	2	0
2	A	501	CAA	1	0
2	L	511	CAA	2	0

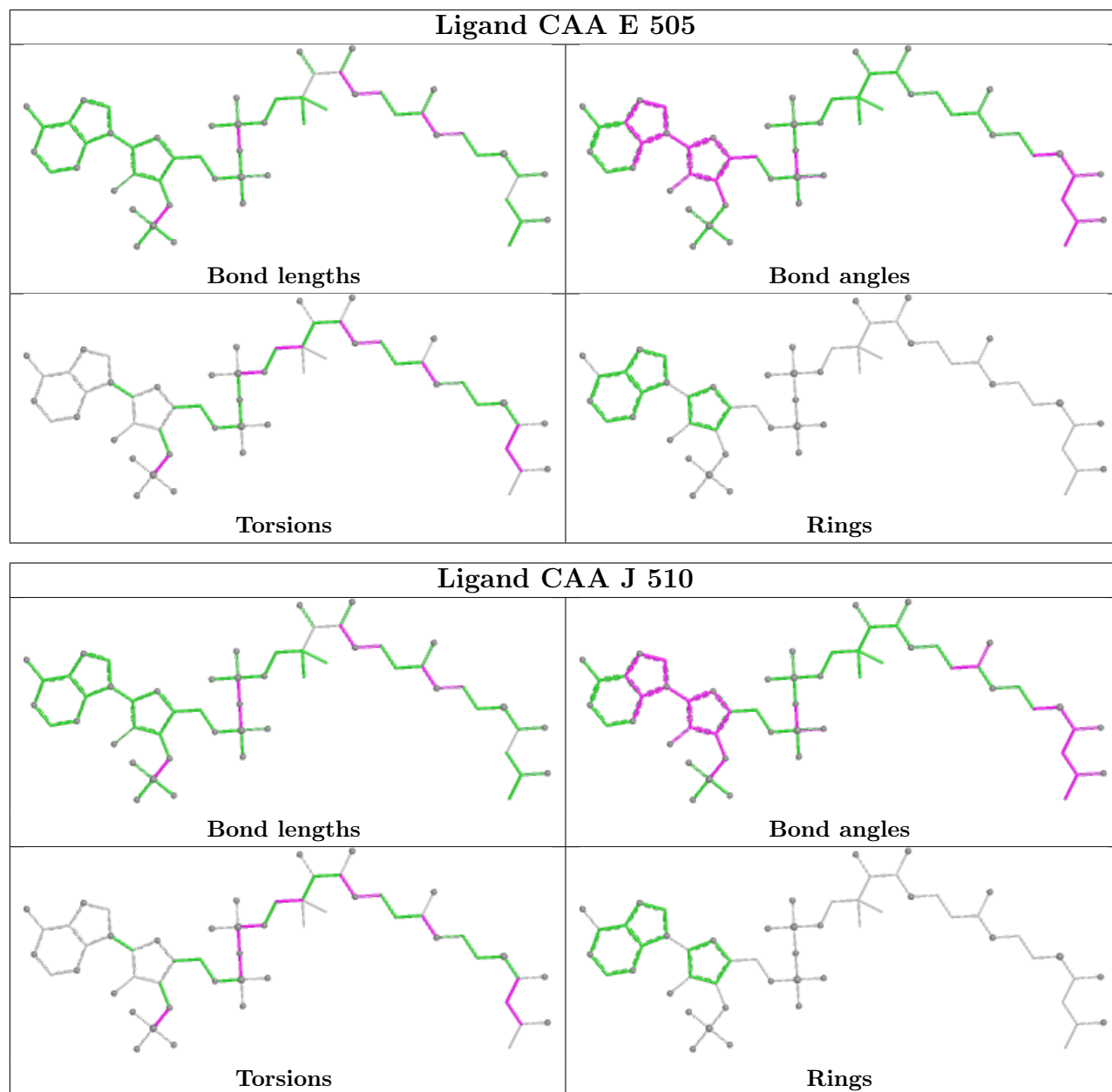
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

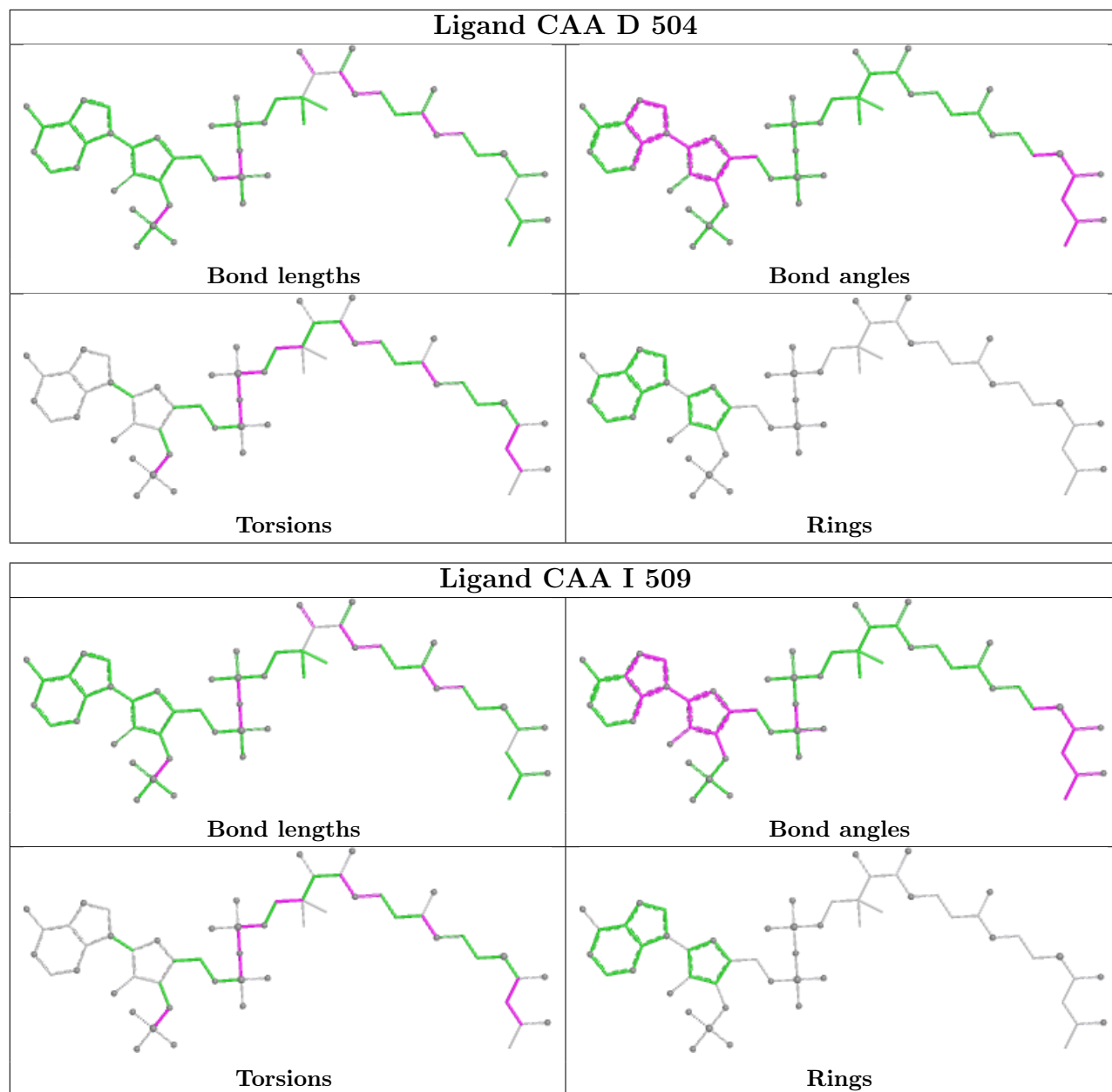
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

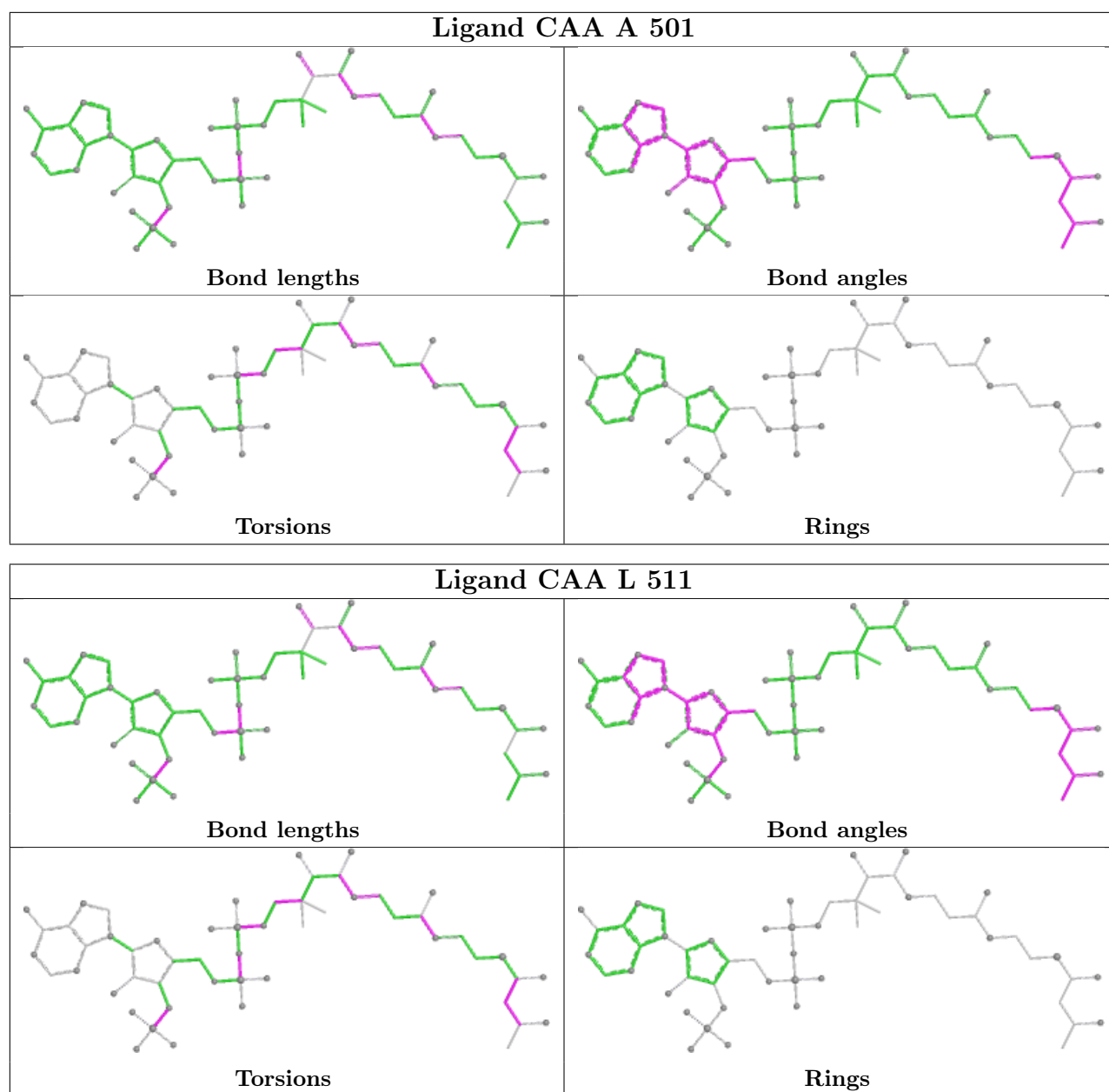












5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.