



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:28 PM UTC

PDB ID : 7WDW / pdb_00007wdw
Title : DsyB in complex with SAH and MTHB
Authors : Li, C.Y.
Deposited on : 2021-12-22
Resolution : 2.39 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

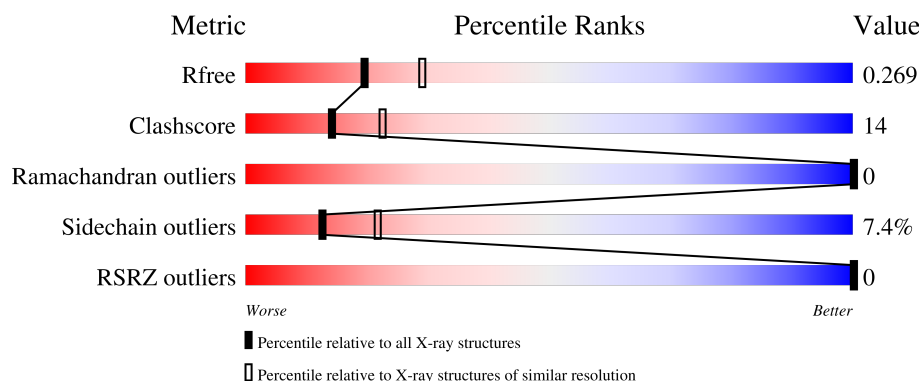
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	343	
1	B	343	
1	C	343	
1	D	343	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TRS	D	402	-	X	-	-

2 Entry composition [i](#)

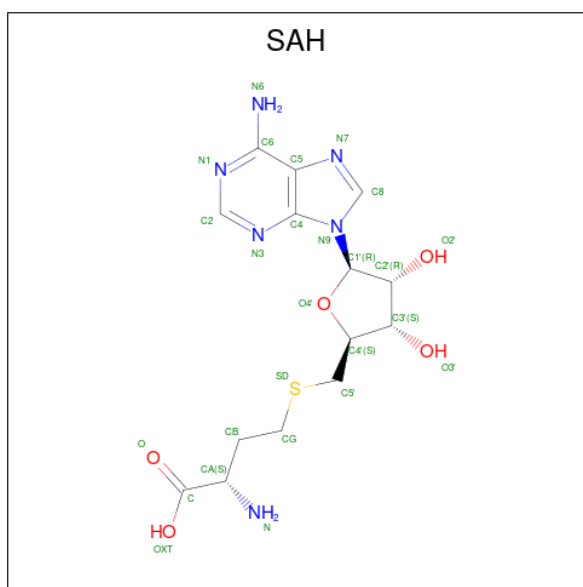
There are 5 unique types of molecules in this entry. The entry contains 10644 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DSYB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2538	1615	426	488	9			
1	B	336	Total	C	N	O	S	0	2	0
			2555	1624	428	494	9			
1	C	336	Total	C	N	O	S	0	3	0
			2555	1625	427	494	9			
1	D	336	Total	C	N	O	S	0	0	0
			2538	1615	426	488	9			

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



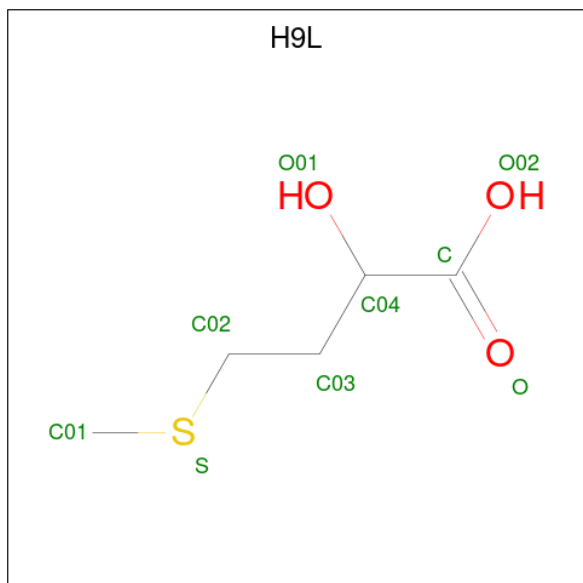
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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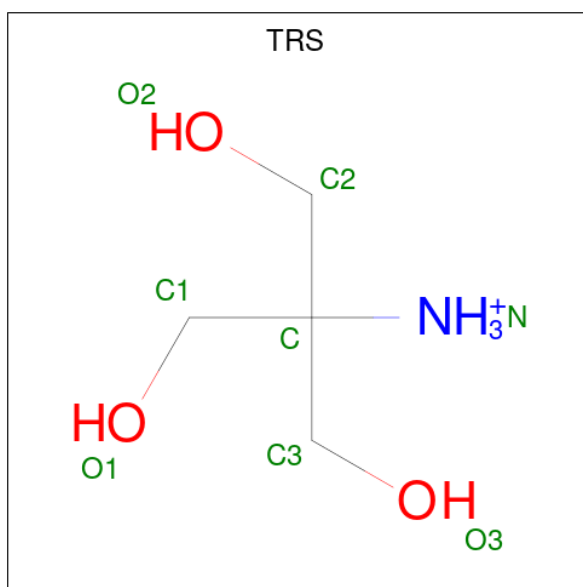
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is 4-methylsulfanyl-2-oxidanyl-butanoic acid (CCD ID: H9L) (formula: $C_5H_{10}O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			9	5	3	1		
3	B	1	Total	C	O	S	0	0
			9	5	3	1		
3	C	1	Total	C	O	S	0	0
			9	5	3	1		
3	D	1	Total	C	O	S	0	0
			9	5	3	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			8	4	1	3		
4	C	1	Total	C	N	O	0	0
			8	4	1	3		
4	D	1	Total	C	N	O	0	0
			8	4	1	3		
4	D	1	Total	C	N	O	0	0
			8	4	1	3		

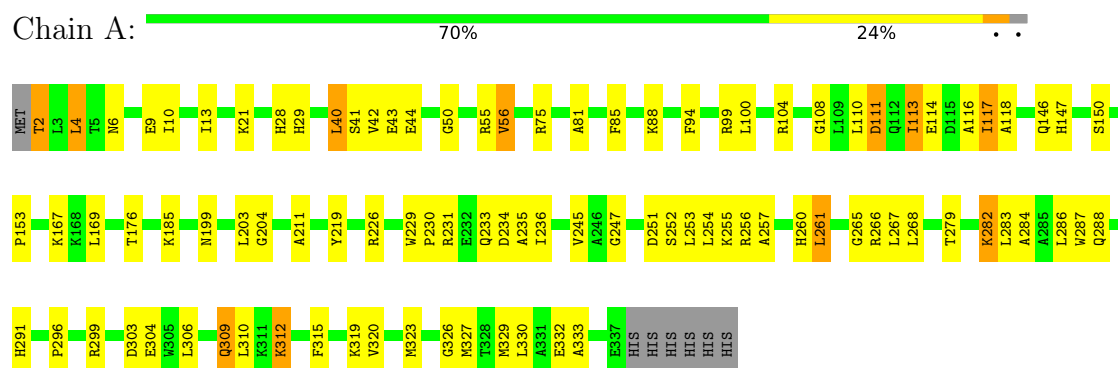
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		
5	B	63	Total	O	0	0
			63	63		
5	C	87	Total	O	0	0
			87	87		
5	D	75	Total	O	0	0
			75	75		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

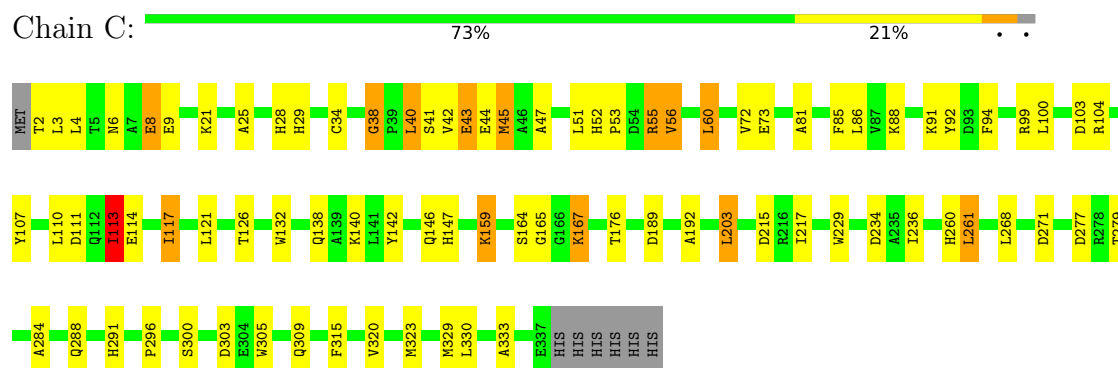
• Molecule 1: DSYB



• Molecule 1: DSYB



• Molecule 1: DSYB



● Molecule 1: DSYB

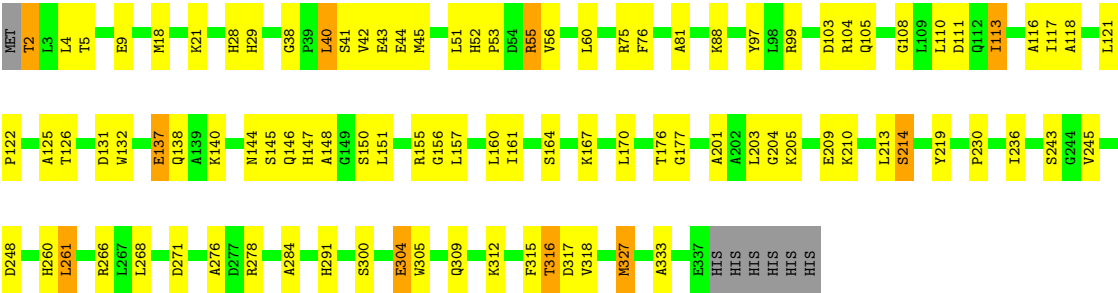
Chain D:

70%

25%

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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.10Å 69.29Å 104.34Å 90.00° 92.19° 90.00°	Depositor
Resolution (Å)	37.16 – 2.39 37.16 – 2.39	Depositor EDS
% Data completeness (in resolution range)	92.3 (37.16-2.39) 99.4 (37.16-2.39)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.187 , 0.268 0.191 , 0.269	Depositor DCC
R_{free} test set	2505 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.006 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10644	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6644e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TRS, H9L, SAH

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	0.49	0/2591	0.83	0/3518
1	B	0.48	0/2608	0.83	2/3541 (0.1%)
1	C	0.53	0/2614	0.83	4/3549 (0.1%)
1	D	0.53	0/2591	0.87	4/3518 (0.1%)
All	All	0.51	0/10404	0.84	10/14126 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	GLY	CA-C-N	5.85	126.15	119.83
1	C	38	GLY	C-N-CA	5.85	126.15	119.83
1	D	271	ASP	N-CA-C	5.79	116.94	108.14
1	D	38	GLY	CA-C-N	5.54	126.76	119.84
1	D	38	GLY	C-N-CA	5.54	126.76	119.84
1	B	118	ALA	N-CA-C	-5.35	105.98	112.88
1	D	318	VAL	CB-CA-C	-5.30	106.18	111.80
1	C	113	ILE	N-CA-CB	5.18	116.95	110.47
1	C	271	ASP	N-CA-C	5.05	115.87	107.73
1	B	113	ILE	CB-CA-C	-5.03	105.36	112.14

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	2538	0	2502	84	0
1	B	2555	0	2510	90	0
1	C	2555	0	2516	77	0
1	D	2538	0	2502	69	0
2	A	26	0	18	2	0
2	B	26	0	18	1	0
2	C	26	0	18	1	0
2	D	26	0	18	1	0
3	A	9	0	0	1	0
3	B	9	0	0	0	0
3	C	9	0	0	3	0
3	D	9	0	0	3	0
4	B	8	0	12	5	0
4	C	8	0	12	4	0
4	D	16	0	24	4	0
5	A	61	0	0	1	0
5	B	63	0	0	0	0
5	C	87	0	0	3	0
5	D	75	0	0	2	0
All	All	10644	0	10150	292	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 14.

All (292) 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:29:HIS:CE1	1:D:117:ILE:HD11	1.88	1.08
1:C:104:ARG:O	4:C:402:TRS:H21	1.61	1.00
1:C:6:ASN:HB2	1:C:9:GLU:HG3	1.42	0.99
1:B:108:GLY:HA3	4:B:402:TRS:H32	1.45	0.97
1:A:21:LYS:HD2	1:D:113:ILE:HD11	1.54	0.90
1:A:309:GLN:HE21	1:A:312:LYS:HE3	1.38	0.89
1:B:278:ARG:HG2	1:B:278:ARG:HH11	1.37	0.88
1:B:226:ARG:HH11	1:B:226:ARG:CG	1.90	0.85
1:B:21:LYS:HE3	1:C:113:ILE:HD11	1.60	0.84
1:B:226:ARG:HH11	1:B:226:ARG:HG2	1.45	0.81
1:D:140:LYS:HA	1:D:203:LEU:HD11	1.62	0.81
1:A:113:ILE:HD11	1:D:21:LYS:HD2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HD21	1:A:13:ILE:HD12	1.63	0.80
1:D:97:TYR:HA	1:D:145:SER:HB3	1.61	0.80
1:A:323:MET:HE2	1:A:330:LEU:HB2	1.64	0.80
1:B:106:MET:HE3	1:B:287:TRP:HZ3	1.48	0.79
1:C:303:ASP:HB3	1:C:329:MET:HE1	1.65	0.78
4:B:402:TRS:H11	1:C:111:ASP:OD2	1.85	0.76
1:C:113:ILE:O	1:C:117:ILE:HG13	1.85	0.76
1:C:9:GLU:OE2	1:D:2:THR:HG22	1.85	0.75
1:A:110:LEU:O	1:A:113:ILE:HG13	1.87	0.75
1:B:147:HIS:HD2	1:B:176:THR:OG1	1.68	0.75
1:B:113:ILE:O	1:B:117:ILE:HG13	1.86	0.75
1:B:113:ILE:HD13	1:C:25:ALA:HB2	1.70	0.74
1:A:147:HIS:HD2	1:A:176:THR:OG1	1.71	0.74
1:B:315:PHE:HB3	1:B:333:ALA:HB1	1.71	0.73
1:A:2:THR:N	1:B:5:THR:HG1	1.88	0.71
1:D:104:ARG:O	4:D:402:TRS:H32	1.90	0.71
1:B:278:ARG:HG2	1:B:278:ARG:NH1	2.06	0.71
1:B:85:PHE:HB3	1:B:94:PHE:HE1	1.56	0.70
1:B:113:ILE:HD11	1:C:21:LYS:HD2	1.71	0.70
1:C:34:CYS:HB2	1:C:45:MET:HE1	1.75	0.68
1:D:156:GLY:O	1:D:160:LEU:HD23	1.93	0.68
1:A:117:ILE:O	1:D:51:LEU:HD22	1.93	0.68
1:B:104:ARG:HA	4:B:402:TRS:H22	1.75	0.68
1:C:320:VAL:HG12	1:C:329:MET:CE	2.24	0.68
1:D:113:ILE:O	1:D:117:ILE:HG13	1.93	0.68
1:A:320:VAL:HG12	1:A:329:MET:HE2	1.76	0.67
1:C:41:SER:OG	1:C:43:GLU:HG2	1.94	0.67
1:C:88:LYS:HE2	1:C:88:LYS:N	2.10	0.67
1:A:257:ALA:HB1	1:A:267:LEU:HD13	1.75	0.67
1:B:305:TRP:CZ2	1:B:309:GLN:HG3	2.30	0.67
1:C:305:TRP:CZ2	1:C:309:GLN:HG3	2.30	0.66
1:D:41:SER:OG	1:D:44:GLU:HG3	1.96	0.66
1:D:108:GLY:HA3	4:D:402:TRS:H11	1.76	0.66
1:D:110:LEU:O	1:D:113:ILE:HG13	1.95	0.66
1:D:147:HIS:HD2	1:D:176:THR:OG1	1.79	0.66
1:B:29:HIS:CE1	1:C:117:ILE:HD11	2.31	0.66
1:A:150:SER:C	1:A:153:PRO:HD2	2.22	0.65
1:B:236:ILE:HG13	1:B:261:LEU:HD13	1.78	0.63
1:B:85:PHE:HB3	1:B:94:PHE:CE1	2.34	0.63
1:A:185:LYS:NZ	1:A:211:ALA:HB1	2.13	0.63
1:B:150:SER:C	1:B:153:PRO:HD2	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:HIS:CD2	1:B:176:THR:OG1	2.50	0.62
1:D:117:ILE:HD12	1:D:118:ALA:N	2.14	0.62
1:A:42:VAL:HG13	1:A:56:VAL:HG22	1.82	0.62
2:C:401:SAH:HB1	2:C:401:SAH:H4'	1.81	0.62
1:A:85:PHE:HB3	1:A:94:PHE:CE1	2.35	0.62
1:C:192:ALA:HB3	1:C:217:ILE:HG12	1.82	0.62
1:D:117:ILE:HD12	1:D:117:ILE:C	2.26	0.61
1:D:209:GLU:HG2	5:D:538:HOH:O	2.00	0.61
1:B:170:LEU:HD21	1:B:229:TRP:HB3	1.82	0.61
1:A:323:MET:HE1	1:A:330:LEU:HD22	1.81	0.61
1:A:284:ALA:O	1:A:288:GLN:HG3	2.01	0.60
1:B:166:GLY:HA2	1:B:189:ASP:HB3	1.82	0.60
1:B:305:TRP:CH2	1:B:309:GLN:HG3	2.36	0.60
1:C:104:ARG:O	4:C:402:TRS:H31	2.02	0.60
1:B:101:GLN:HE21	1:B:145:SER:HB3	1.67	0.60
1:C:38:GLY:O	1:C:40:LEU:HD13	2.01	0.60
1:C:323:MET:HE2	1:C:330:LEU:HB2	1.84	0.60
1:B:29:HIS:CE1	1:C:117:ILE:CD1	2.85	0.59
1:D:140:LYS:HA	1:D:203:LEU:CD1	2.32	0.59
1:A:247:GLY:HA3	1:A:299:ARG:HG2	1.85	0.58
1:D:28:HIS:NE2	1:D:103:ASP:OD2	2.33	0.58
1:A:28:HIS:CE1	1:A:99:ARG:HB2	2.38	0.58
1:C:51:LEU:HB2	1:C:56:VAL:HG12	1.84	0.58
1:B:199:ASN:O	1:B:203:LEU:HG	2.03	0.58
1:A:88:LYS:HD2	5:A:558:HOH:O	2.04	0.57
1:B:21:LYS:HD3	1:B:107:TYR:CE2	2.40	0.57
1:D:105:GLN:HA	4:D:402:TRS:H32	1.86	0.57
1:D:209:GLU:OE1	1:D:214:SER:HB2	2.04	0.57
1:A:4:LEU:HD21	1:A:13:ILE:CD1	2.34	0.56
1:A:50:GLY:O	4:D:403:TRS:H31	2.05	0.56
1:B:284:ALA:O	1:B:288:GLN:HG3	2.05	0.56
1:C:147:HIS:HD2	1:C:176:THR:OG1	1.89	0.56
1:B:113:ILE:HA	1:B:116:ALA:HB3	1.86	0.56
1:B:28:HIS:HA	1:B:99:ARG:HH11	1.70	0.56
1:C:277:ASP:OD1	1:C:279:THR:HG22	2.06	0.56
1:B:55:ARG:HD3	1:C:296:PRO:O	2.06	0.56
1:C:2:THR:HG23	1:D:9:GLU:OE2	2.06	0.55
1:D:52:HIS:O	1:D:56:VAL:HG22	2.06	0.55
1:A:169:LEU:HD12	1:A:235:ALA:O	2.06	0.55
1:A:100:LEU:O	1:A:104:ARG:HB2	2.07	0.55
1:A:204:GLY:HA3	1:A:219:TYR:OH	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LEU:HB2	1:B:56:VAL:CG1	2.36	0.55
1:B:4:LEU:HD11	1:B:13:ILE:HD12	1.89	0.55
1:C:110:LEU:O	1:C:113:ILE:HG13	2.06	0.55
1:A:81:ALA:HB2	1:D:5:THR:CA	2.37	0.54
1:C:320:VAL:HG12	1:C:329:MET:HE3	1.89	0.54
1:D:146:GLN:HE22	3:D:404:H9L:C02	2.20	0.54
1:D:164:SER:O	1:D:167:LYS:HD3	2.07	0.54
1:A:113:ILE:O	1:A:117:ILE:HG13	2.07	0.54
1:B:315:PHE:CB	1:B:333:ALA:HB1	2.38	0.54
1:B:117:ILE:HA	1:C:55:ARG:HG2	1.88	0.54
1:A:309:GLN:NE2	1:A:312:LYS:HE3	2.17	0.54
1:A:310:LEU:O	1:A:315:PHE:HB2	2.08	0.54
1:C:28:HIS:CE1	1:C:99:ARG:HB2	2.43	0.53
1:C:140:LYS:HA	1:C:203:LEU:HD11	1.90	0.53
1:C:167:LYS:HG2	1:C:234:ASP:CG	2.34	0.53
1:A:287:TRP:CE2	1:D:18:MET:HE1	2.43	0.53
1:A:41:SER:OG	1:A:43:GLU:HG2	2.09	0.53
1:B:316:THR:HG22	1:B:317:ASP:N	2.24	0.53
1:B:42:VAL:HG13	1:B:56:VAL:CG2	2.39	0.53
2:D:401:SAH:HB1	2:D:401:SAH:H4'	1.90	0.52
1:B:55:ARG:HG2	1:C:117:ILE:HA	1.90	0.52
1:B:28:HIS:CE1	1:B:99:ARG:HB2	2.44	0.52
1:A:116:ALA:C	1:A:118:ALA:H	2.18	0.52
1:D:122:PRO:HD2	1:D:125:ALA:HB2	1.91	0.52
1:D:146:GLN:OE1	3:D:404:H9L:C02	2.57	0.52
1:B:195:VAL:HG22	1:B:220:VAL:HB	1.92	0.52
1:A:44:GLU:OE2	1:A:75:ARG:NH2	2.43	0.51
1:D:147:HIS:CD2	1:D:176:THR:OG1	2.60	0.51
1:D:209:GLU:CD	1:D:214:SER:OG	2.52	0.51
1:A:150:SER:O	1:A:153:PRO:HD2	2.11	0.51
1:A:255:LYS:NZ	1:A:309:GLN:HE22	2.07	0.51
1:D:305:TRP:CZ2	1:D:309:GLN:HG3	2.45	0.51
1:A:147:HIS:CD2	1:A:176:THR:OG1	2.57	0.51
1:A:320:VAL:HG12	1:A:329:MET:CE	2.39	0.51
1:A:247:GLY:CA	1:A:299:ARG:HG2	2.40	0.51
1:C:126:THR:CG2	1:C:132:TRP:HB2	2.41	0.51
1:C:126:THR:HG21	1:C:132:TRP:HB2	1.93	0.51
1:D:315:PHE:HB3	1:D:333:ALA:HB1	1.91	0.51
1:C:315:PHE:HB3	1:C:333:ALA:HB1	1.93	0.51
1:B:87:VAL:O	1:B:93:ASP:HB2	2.11	0.51
1:A:146:GLN:NE2	2:A:401:SAH:HG1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LYS:HE3	1:A:332:GLU:CD	2.37	0.51
1:B:5:THR:C	1:C:81:ALA:HB2	2.36	0.51
1:D:276:ALA:HB2	1:D:304:GLU:HB2	1.94	0.51
1:D:316:THR:HG22	1:D:317:ASP:H	1.76	0.51
1:A:284:ALA:HB2	1:A:327:MET:O	2.11	0.50
1:A:236:ILE:HD12	1:A:261:LEU:HD13	1.94	0.50
1:A:255:LYS:H	1:A:255:LYS:HD2	1.76	0.50
1:D:230:PRO:O	1:D:260:HIS:HD2	1.95	0.50
2:B:401:SAH:HB1	2:B:401:SAH:H4'	1.94	0.50
1:B:51:LEU:HB2	1:B:56:VAL:HG12	1.94	0.50
1:D:42:VAL:HG13	1:D:56:VAL:HG23	1.93	0.50
1:D:53:PRO:HA	1:D:56:VAL:CG2	2.41	0.50
1:C:85:PHE:HB3	1:C:94:PHE:CE1	2.47	0.50
1:C:147:HIS:CD2	1:C:176:THR:OG1	2.64	0.50
1:C:291:HIS:CE1	3:C:403:H9L:C01	2.95	0.50
1:B:35:LEU:HD22	1:B:76:PHE:O	2.12	0.50
1:B:110:LEU:O	1:B:113:ILE:HG13	2.12	0.50
1:D:236:ILE:HD12	1:D:261:LEU:HD13	1.93	0.50
1:A:40:LEU:HG	1:A:44:GLU:HB3	1.92	0.49
1:C:121:LEU:HD12	1:C:296:PRO:HG3	1.94	0.49
1:A:6:ASN:HB2	1:A:9:GLU:HG3	1.93	0.49
1:C:104:ARG:HA	4:C:402:TRS:H31	1.94	0.49
1:D:28:HIS:CE1	1:D:99:ARG:HB2	2.47	0.49
1:A:108:GLY:O	1:A:111:ASP:HB2	2.13	0.49
1:A:199:ASN:O	1:A:203:LEU:HG	2.13	0.49
1:D:116:ALA:HB2	1:D:121:LEU:HD21	1.93	0.49
1:A:185:LYS:HZ1	1:A:211:ALA:HB1	1.76	0.49
1:A:282:LYS:O	1:A:286:LEU:HG	2.12	0.49
1:A:117:ILE:CD1	1:D:29:HIS:CE1	2.96	0.49
1:A:229:TRP:HB2	1:A:260:HIS:CD2	2.48	0.49
1:A:315:PHE:CD1	1:A:333:ALA:HB1	2.48	0.48
1:B:236:ILE:HG13	1:B:261:LEU:CD1	2.42	0.48
1:A:117:ILE:HD11	1:D:29:HIS:CE1	2.49	0.48
1:C:305:TRP:CE2	1:C:309:GLN:HG3	2.48	0.48
1:A:255:LYS:HZ3	1:A:309:GLN:HE22	1.62	0.48
1:C:47:ALA:N	5:C:501:HOH:O	2.46	0.48
1:A:251:ASP:O	1:A:255:LYS:HD2	2.13	0.48
1:A:113:ILE:HD12	1:A:114:GLU:H	1.79	0.47
1:B:26:ALA:HB1	1:B:31:VAL:HB	1.97	0.47
1:B:226:ARG:CG	1:B:226:ARG:NH1	2.57	0.47
1:B:335:ARG:HG3	1:B:336:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:HB3	1:D:45:MET:HG2	1.97	0.47
1:C:165:GLY:O	1:C:189:ASP:HB2	2.14	0.47
1:D:204:GLY:HA3	1:D:219:TYR:OH	2.14	0.47
1:B:110:LEU:HD13	1:B:290:GLN:HA	1.96	0.47
1:B:150:SER:O	1:B:153:PRO:HD2	2.14	0.47
1:A:150:SER:OG	2:A:401:SAH:OXT	2.28	0.46
1:C:91:LYS:HE3	1:C:92:TYR:CZ	2.50	0.46
1:C:229:TRP:HB2	1:C:260:HIS:CD2	2.50	0.46
1:B:226:ARG:HH11	1:B:226:ARG:HG3	1.76	0.46
1:C:45:MET:HA	1:C:45:MET:HE2	1.97	0.46
1:A:296:PRO:O	1:D:55:ARG:HD3	2.16	0.46
1:B:278:ARG:NH1	1:B:278:ARG:CG	2.73	0.46
1:C:85:PHE:O	1:C:86:LEU:HD23	2.15	0.46
1:B:204:GLY:HA3	1:B:219:TYR:OH	2.15	0.46
1:A:266:ARG:HG3	1:A:333:ALA:O	2.16	0.46
1:B:226:ARG:NH1	1:B:226:ARG:HG3	2.31	0.46
1:A:319:LYS:HE3	1:A:332:GLU:OE2	2.16	0.46
1:D:177:GLY:HA2	5:D:505:HOH:O	2.16	0.46
1:A:42:VAL:HG13	1:A:56:VAL:CG2	2.45	0.45
1:C:99:ARG:O	1:C:103:ASP:HB3	2.16	0.45
1:A:113:ILE:HD12	1:A:114:GLU:N	2.31	0.45
1:B:111:ASP:OD2	4:C:402:TRS:H12	2.16	0.45
1:C:52:HIS:O	1:C:56:VAL:HG13	2.17	0.45
1:B:107:TYR:CD1	1:B:107:TYR:C	2.95	0.45
1:C:132:TRP:NE1	1:C:138:GLN:HB3	2.31	0.45
1:C:159:LYS:HB2	1:C:159:LYS:HE2	1.62	0.45
1:D:201:ALA:O	1:D:205:LYS:HG3	2.16	0.45
1:B:78:ASN:HB2	1:B:83[B]:GLU:HG2	1.97	0.45
1:D:4:LEU:HD22	1:D:9:GLU:HB3	1.98	0.45
1:A:116:ALA:C	1:A:118:ALA:N	2.73	0.45
1:A:261:LEU:HG	1:A:265:GLY:HA3	1.98	0.45
1:B:133:PHE:CD1	1:B:139:ALA:HA	2.52	0.45
1:B:159:LYS:O	1:B:159:LYS:HG3	2.15	0.45
1:C:164:SER:O	1:C:167:LYS:HD2	2.17	0.45
1:D:137:GLU:HG3	1:D:138:GLN:N	2.32	0.45
1:A:252:SER:O	1:A:256:ARG:HG3	2.17	0.44
1:A:312:LYS:O	1:A:312:LYS:HG3	2.17	0.44
1:B:109:LEU:HD23	1:B:109:LEU:HA	1.65	0.44
1:A:10:ILE:HD11	1:D:81:ALA:HB1	2.00	0.44
1:A:303:ASP:OD1	1:A:304:GLU:N	2.51	0.44
1:D:243:SER:HB3	1:D:291:HIS:ND1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:LEU:HB3	1:D:76:PHE:CE2	2.53	0.44
1:A:231:ARG:HG2	1:A:260:HIS:CD2	2.53	0.44
1:B:261:LEU:HG	1:B:265:GLY:HA3	2.00	0.44
1:C:88:LYS:HE3	5:C:546:HOH:O	2.18	0.44
1:C:291:HIS:HE1	3:C:403:H9L:C01	2.30	0.44
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.71	0.44
1:C:140:LYS:HG2	1:C:203:LEU:HD11	2.00	0.44
1:D:284:ALA:HB2	1:D:327:MET:O	2.17	0.44
1:B:81:ALA:HB2	1:C:4:LEU:C	2.43	0.43
1:B:104:ARG:CA	4:B:402:TRS:H22	2.44	0.43
1:B:106:MET:HE3	1:B:287:TRP:CZ3	2.39	0.43
1:B:316:THR:O	1:B:317:ASP:HB2	2.17	0.43
1:D:213:LEU:HD23	1:D:213:LEU:HA	1.85	0.43
1:A:230:PRO:HB2	1:A:233:GLN:NE2	2.33	0.43
1:A:167:LYS:HG2	1:A:234:ASP:CG	2.42	0.43
1:B:323:MET:HE3	1:B:330:LEU:HB2	2.00	0.43
1:C:60:LEU:N	1:C:60:LEU:CD2	2.80	0.43
1:D:236:ILE:CD1	1:D:261:LEU:HD13	2.47	0.43
1:B:117:ILE:CD1	1:C:29:HIS:CE1	3.01	0.43
1:C:284:ALA:O	1:C:288:GLN:HG3	2.19	0.43
1:A:306:LEU:O	1:A:310:LEU:HG	2.19	0.43
1:C:236:ILE:HG13	1:C:261:LEU:HD13	2.00	0.43
1:D:157:LEU:O	1:D:161:ILE:HG12	2.18	0.43
1:B:113:ILE:O	1:B:114:GLU:C	2.61	0.42
1:A:283:LEU:HB2	1:A:326:GLY:O	2.18	0.42
1:C:41:SER:OG	1:C:44:GLU:HG3	2.19	0.42
1:D:56:VAL:O	1:D:60:LEU:HD23	2.18	0.42
1:B:42:VAL:HG13	1:B:56:VAL:HG23	2.02	0.42
1:B:119:ASN:HD21	1:C:55:ARG:HH11	1.68	0.42
1:D:126:THR:CG2	1:D:132:TRP:HB2	2.49	0.42
1:B:261:LEU:HD12	1:B:261:LEU:HA	1.81	0.42
1:C:6:ASN:HB2	1:C:9:GLU:CG	2.31	0.42
1:C:8:GLU:O	1:C:8:GLU:HG3	2.19	0.42
1:C:21:LYS:HE2	1:C:107:TYR:CG	2.54	0.42
1:D:278:ARG:HH12	1:D:300:SER:CB	2.32	0.42
1:B:88:LYS:HA	1:B:93:ASP:OD2	2.19	0.42
1:B:192:ALA:HB3	1:B:217:ILE:HG12	2.02	0.42
1:B:296:PRO:O	1:C:55:ARG:HD3	2.19	0.42
1:B:335:ARG:HG3	1:B:336:PRO:CD	2.50	0.42
1:D:170:LEU:O	1:D:236:ILE:HA	2.19	0.42
1:B:5:THR:CA	1:C:81:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:SER:O	1:B:83[A]:GLU:HG3	2.20	0.42
1:A:230:PRO:HB2	1:A:233:GLN:HE21	1.84	0.42
1:A:254:LEU:HD12	1:A:309:GLN:OE1	2.19	0.42
1:A:113:ILE:O	1:A:114:GLU:C	2.63	0.41
1:B:21:LYS:HE2	1:C:110:LEU:O	2.20	0.41
1:B:28:HIS:HA	1:B:99:ARG:NH1	2.34	0.41
1:B:130:ALA:HB2	1:B:197:PHE:CZ	2.55	0.41
1:C:142:TYR:CD1	1:C:142:TYR:C	2.98	0.41
1:D:151:LEU:O	1:D:155:ARG:HG3	2.20	0.41
1:A:81:ALA:HB2	1:D:5:THR:C	2.46	0.41
1:A:283:LEU:HD13	1:A:327:MET:HE2	2.02	0.41
1:C:113:ILE:O	1:C:114:GLU:C	2.64	0.41
1:A:9:GLU:OE2	1:B:2:THR:HG23	2.21	0.41
1:A:113:ILE:HA	1:A:116:ALA:HB3	2.03	0.41
1:C:146:GLN:HE22	3:C:403:H9L:C03	2.33	0.41
1:B:104:ARG:C	4:B:402:TRS:H22	2.45	0.41
1:D:210:LYS:HG3	1:D:210:LYS:O	2.20	0.41
1:C:47:ALA:HB2	5:C:501:HOH:O	2.21	0.41
1:C:52:HIS:CG	1:C:53:PRO:HD2	2.56	0.41
1:B:274:VAL:HG23	1:B:275:THR:O	2.21	0.41
1:C:100:LEU:O	1:C:104:ARG:HB2	2.20	0.41
1:D:51:LEU:HB2	1:D:56:VAL:HG13	2.02	0.41
1:A:236:ILE:CD1	1:A:261:LEU:HD13	2.51	0.41
1:B:167:LYS:HD3	1:B:234:ASP:HB3	2.03	0.41
1:B:175:GLY:HA2	1:B:200:VAL:HG11	2.02	0.40
1:C:110:LEU:HD12	1:C:110:LEU:HA	1.89	0.40
1:A:291:HIS:NE2	3:A:402:H9L:C01	2.83	0.40
1:B:21:LYS:CE	1:C:113:ILE:HD11	2.41	0.40
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.93	0.40
1:D:117:ILE:C	1:D:117:ILE:CD1	2.94	0.40
1:D:140:LYS:HG3	1:D:144:ASN:OD1	2.22	0.40
1:D:145:SER:O	1:D:148:ALA:N	2.54	0.40
1:D:146:GLN:NE2	3:D:404:H9L:C02	2.84	0.40
1:B:99:ARG:O	1:B:103:ASP:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	334/343 (97%)	321 (96%)	13 (4%)	0	100	100
1	B	336/343 (98%)	325 (97%)	11 (3%)	0	100	100
1	C	337/343 (98%)	320 (95%)	17 (5%)	0	100	100
1	D	334/343 (97%)	320 (96%)	14 (4%)	0	100	100
All	All	1341/1372 (98%)	1286 (96%)	55 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/267 (97%)	244 (94%)	16 (6%)	16	29
1	B	262/267 (98%)	242 (92%)	20 (8%)	12	21
1	C	263/267 (98%)	242 (92%)	21 (8%)	11	19
1	D	260/267 (97%)	239 (92%)	21 (8%)	11	18
All	All	1045/1068 (98%)	967 (92%)	78 (8%)	13	21

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	4	LEU

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Mol	Chain	Res	Type
1	A	40	LEU
1	A	55	ARG
1	A	56	VAL
1	A	111	ASP
1	A	113	ILE
1	A	117	ILE
1	A	226	ARG
1	A	245	VAL
1	A	261	LEU
1	A	268	LEU
1	A	279	THR
1	A	282	LYS
1	A	309	GLN
1	A	312	LYS
1	B	3	LEU
1	B	8	GLU
1	B	10	ILE
1	B	40	LEU
1	B	43	GLU
1	B	55	ARG
1	B	113	ILE
1	B	117	ILE
1	B	127	SER
1	B	141	LEU
1	B	144	ASN
1	B	145	SER
1	B	210	LYS
1	B	226	ARG
1	B	243	SER
1	B	245	VAL
1	B	261	LEU
1	B	266	ARG
1	B	282	LYS
1	B	317	ASP
1	C	3	LEU
1	C	8	GLU
1	C	40	LEU
1	C	42	VAL
1	C	43	GLU
1	C	45	MET
1	C	55	ARG
1	C	56	VAL

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Mol	Chain	Res	Type
1	C	60	LEU
1	C	72	VAL
1	C	73	GLU
1	C	113	ILE
1	C	117	ILE
1	C	159	LYS
1	C	167	LYS
1	C	203	LEU
1	C	215[A]	ASP
1	C	215[B]	ASP
1	C	261	LEU
1	C	268	LEU
1	C	300	SER
1	D	2	THR
1	D	40	LEU
1	D	43	GLU
1	D	55	ARG
1	D	75	ARG
1	D	88	LYS
1	D	111	ASP
1	D	113	ILE
1	D	131	ASP
1	D	137	GLU
1	D	150	SER
1	D	214	SER
1	D	245	VAL
1	D	248	ASP
1	D	261	LEU
1	D	266	ARG
1	D	268	LEU
1	D	304	GLU
1	D	312	LYS
1	D	316	THR
1	D	327	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	112	GLN
1	A	144	ASN
1	A	147	HIS

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Mol	Chain	Res	Type
1	A	233	GLN
1	A	290	GLN
1	A	309	GLN
1	B	29	HIS
1	B	57	GLN
1	B	101	GLN
1	B	144	ASN
1	B	147	HIS
1	C	29	HIS
1	C	101	GLN
1	C	146	GLN
1	C	147	HIS
1	C	260	HIS
1	C	291	HIS
1	D	29	HIS
1	D	147	HIS
1	D	233	GLN
1	D	260	HIS
1	D	290	GLN

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	$\# Z > 2$
3	H9L	B	403	-	8,8,8	0.90	0	8,9,9	1.53	1 (12%)
2	SAH	C	401	-	27,28,28	1.61	4 (14%)	36,40,40	2.36	12 (33%)
4	TRS	B	402	-	7,7,7	1.13	0	9,9,9	2.20	3 (33%)
4	TRS	C	402	-	7,7,7	1.02	0	9,9,9	2.10	3 (33%)
3	H9L	C	403	-	8,8,8	0.93	0	8,9,9	1.56	1 (12%)
2	SAH	D	401	-	27,28,28	1.73	5 (18%)	36,40,40	2.20	10 (27%)
3	H9L	D	404	-	8,8,8	0.85	0	8,9,9	1.68	2 (25%)
2	SAH	A	401	-	27,28,28	1.71	4 (14%)	36,40,40	2.26	11 (30%)
2	SAH	B	401	-	27,28,28	1.70	6 (22%)	36,40,40	2.23	10 (27%)
3	H9L	A	402	-	8,8,8	0.87	0	8,9,9	1.57	1 (12%)
4	TRS	D	403	-	7,7,7	1.09	0	9,9,9	1.97	3 (33%)
4	TRS	D	402	-	7,7,7	1.15	0	9,9,9	1.72	3 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H9L	B	403	-	-	0/8/8/8	-
2	SAH	C	401	-	-	1/15/31/31	0/3/3/3
4	TRS	B	402	-	-	5/9/9/9	-
4	TRS	C	402	-	-	5/9/9/9	-
3	H9L	C	403	-	-	7/8/8/8	-
2	SAH	D	401	-	-	1/15/31/31	0/3/3/3
3	H9L	D	404	-	-	7/8/8/8	-
2	SAH	A	401	-	-	0/15/31/31	0/3/3/3
2	SAH	B	401	-	-	2/15/31/31	0/3/3/3
3	H9L	A	402	-	-	6/8/8/8	-
4	TRS	D	403	-	-	4/9/9/9	-
4	TRS	D	402	-	-	9/9/9/9	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	SAH	C6-N6	6.06	1.49	1.34
2	D	401	SAH	C6-N6	5.91	1.49	1.34
2	C	401	SAH	C6-N6	5.88	1.49	1.34
2	B	401	SAH	C6-N6	5.80	1.49	1.34
2	D	401	SAH	O3'-C3'	-3.11	1.35	1.43
2	C	401	SAH	O3'-C3'	-2.89	1.35	1.43
2	B	401	SAH	C3'-C4'	-2.89	1.45	1.53
2	A	401	SAH	O3'-C3'	-2.88	1.35	1.43
2	A	401	SAH	C3'-C4'	-2.87	1.45	1.53
2	B	401	SAH	O3'-C3'	-2.83	1.36	1.43
2	D	401	SAH	C3'-C4'	-2.64	1.46	1.53
2	A	401	SAH	C5'-C4'	-2.43	1.43	1.52
2	C	401	SAH	C3'-C4'	-2.34	1.47	1.53
2	D	401	SAH	C5-N7	-2.26	1.35	1.39
2	B	401	SAH	C5'-C4'	-2.18	1.44	1.52
2	C	401	SAH	C5'-C4'	-2.13	1.44	1.52
2	B	401	SAH	C2'-C3'	-2.09	1.47	1.53
2	D	401	SAH	C5'-C4'	-2.05	1.44	1.52
2	B	401	SAH	C2'-C1'	-2.04	1.47	1.53

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	SAH	N3-C2-N1	-5.49	120.26	128.58
2	A	401	SAH	C5-C4-N3	-5.46	119.20	126.72
2	B	401	SAH	C5-C4-N3	-5.43	119.24	126.72
2	C	401	SAH	C5-C4-N3	-5.27	119.45	126.72
2	D	401	SAH	C5-C4-N3	-5.07	119.73	126.72
2	D	401	SAH	N3-C4-N9	4.58	134.95	127.17
2	B	401	SAH	N9-C8-N7	-4.55	107.48	113.94
2	A	401	SAH	N9-C8-N7	-4.52	107.52	113.94
2	C	401	SAH	N9-C8-N7	-4.51	107.54	113.94
2	D	401	SAH	N3-C2-N1	-4.46	121.83	128.58
2	B	401	SAH	N3-C4-N9	4.46	134.75	127.17
4	B	402	TRS	O3-C3-C	4.33	122.94	110.88
2	A	401	SAH	N3-C2-N1	-4.33	122.03	128.58
2	B	401	SAH	N3-C2-N1	-4.20	122.22	128.58
2	A	401	SAH	N3-C4-N9	4.13	134.18	127.17
2	C	401	SAH	N3-C4-N9	4.11	134.15	127.17
2	C	401	SAH	C4-N9-C8	4.06	110.00	105.74
2	B	401	SAH	C4-N9-C8	4.03	109.97	105.74
2	C	401	SAH	C2-N3-C4	4.03	121.67	111.83
2	D	401	SAH	N9-C8-N7	-4.00	108.26	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SAH	C5-N7-C8	3.98	109.71	103.45
2	D	401	SAH	C4-N9-C8	3.96	109.89	105.74
4	B	402	TRS	O2-C2-C	3.85	121.61	110.88
2	A	401	SAH	C4-N9-C8	3.84	109.77	105.74
2	B	401	SAH	C5-N7-C8	3.80	109.42	103.45
4	D	403	TRS	O1-C1-C	3.69	121.17	110.88
2	A	401	SAH	C4-C5-N7	-3.68	106.38	110.58
2	C	401	SAH	C5-N7-C8	3.60	109.11	103.45
4	C	402	TRS	O3-C3-C	3.51	120.66	110.88
3	D	404	H9L	O02-C-C04	3.46	120.06	112.74
2	A	401	SAH	C2-N3-C4	3.44	120.24	111.83
4	D	402	TRS	O3-C3-C	3.44	120.46	110.88
2	D	401	SAH	O4'-C1'-N9	3.44	114.69	108.09
4	D	403	TRS	O3-C3-C	3.31	120.10	110.88
2	B	401	SAH	C2-N3-C4	3.28	119.85	111.83
3	C	403	H9L	O02-C-C04	3.27	119.65	112.74
3	A	402	H9L	O02-C-C04	3.23	119.58	112.74
4	C	402	TRS	O1-C1-C	3.18	119.75	110.88
4	C	402	TRS	O2-C2-C	3.18	119.74	110.88
2	C	401	SAH	C4-C5-N7	-3.17	106.96	110.58
2	D	401	SAH	C2-N3-C4	3.13	119.49	111.83
3	B	403	H9L	O02-C-C04	3.13	119.36	112.74
2	B	401	SAH	O4'-C1'-N9	3.07	113.99	108.09
2	D	401	SAH	C5-N7-C8	3.05	108.24	103.45
2	B	401	SAH	C4-C5-N7	-3.04	107.11	110.58
2	B	401	SAH	C5'-SD-CG	2.96	111.06	102.26
2	C	401	SAH	CB-CG-SD	2.86	119.83	113.45
2	A	401	SAH	C5'-C4'-C3'	-2.76	108.15	115.06
4	D	403	TRS	O2-C2-C	2.75	118.53	110.88
2	C	401	SAH	O4'-C1'-N9	2.71	113.30	108.09
2	A	401	SAH	C5'-SD-CG	2.67	110.20	102.26
2	D	401	SAH	C5'-C4'-C3'	-2.65	108.44	115.06
4	B	402	TRS	O1-C1-C	2.62	118.19	110.88
2	C	401	SAH	C5'-C4'-C3'	-2.49	108.84	115.06
4	D	402	TRS	O2-C2-C	2.39	117.52	110.88
2	A	401	SAH	CB-CG-SD	2.24	118.44	113.45
4	D	402	TRS	O1-C1-C	2.19	116.97	110.88
2	C	401	SAH	OXT-C-O	-2.12	119.26	124.08
3	D	404	H9L	C01-S-C02	2.08	111.08	100.32
2	D	401	SAH	C4-C5-N7	-2.01	108.29	110.58

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	SAH	C-CA-CB-CG
2	D	401	SAH	C-CA-CB-CG
3	C	403	H9L	O02-C-C04-O01
3	C	403	H9L	O-C-C04-O01
3	D	404	H9L	C02-C03-C04-O01
4	B	402	TRS	C1-C-C2-O2
4	B	402	TRS	C3-C-C2-O2
4	B	402	TRS	N-C-C2-O2
4	C	402	TRS	N-C-C1-O1
4	D	402	TRS	N-C-C1-O1
4	D	402	TRS	C1-C-C2-O2
4	D	402	TRS	C3-C-C2-O2
4	D	402	TRS	N-C-C2-O2
4	D	402	TRS	N-C-C3-O3
4	D	403	TRS	C1-C-C2-O2
4	D	403	TRS	C3-C-C2-O2
4	D	403	TRS	N-C-C2-O2
3	A	402	H9L	S-C02-C03-C04
3	C	403	H9L	S-C02-C03-C04
4	D	402	TRS	C2-C-C1-O1
4	D	402	TRS	C1-C-C3-O3
3	D	404	H9L	C03-C02-S-C01
3	A	402	H9L	O02-C-C04-O01
3	A	402	H9L	O-C-C04-O01
3	A	402	H9L	C03-C02-S-C01
3	C	403	H9L	O02-C-C04-C03
3	C	403	H9L	O-C-C04-C03
4	C	402	TRS	C2-C-C1-O1
3	C	403	H9L	C03-C02-S-C01
3	D	404	H9L	S-C02-C03-C04
2	B	401	SAH	C3'-C4'-C5'-SD
4	B	402	TRS	C2-C-C3-O3
4	C	402	TRS	C1-C-C2-O2
4	D	402	TRS	C3-C-C1-O1
4	D	402	TRS	C2-C-C3-O3
2	B	401	SAH	O4'-C4'-C5'-SD
3	D	404	H9L	C02-C03-C04-C
3	A	402	H9L	O-C-C04-C03
4	D	403	TRS	N-C-C3-O3
3	D	404	H9L	O02-C-C04-O01
3	D	404	H9L	O-C-C04-O01
4	B	402	TRS	C1-C-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	402	TRS	C3-C-C1-O1
4	C	402	TRS	C3-C-C2-O2
3	A	402	H9L	O02-C-C04-C03
3	C	403	H9L	C02-C03-C04-O01
3	D	404	H9L	O-C-C04-C03

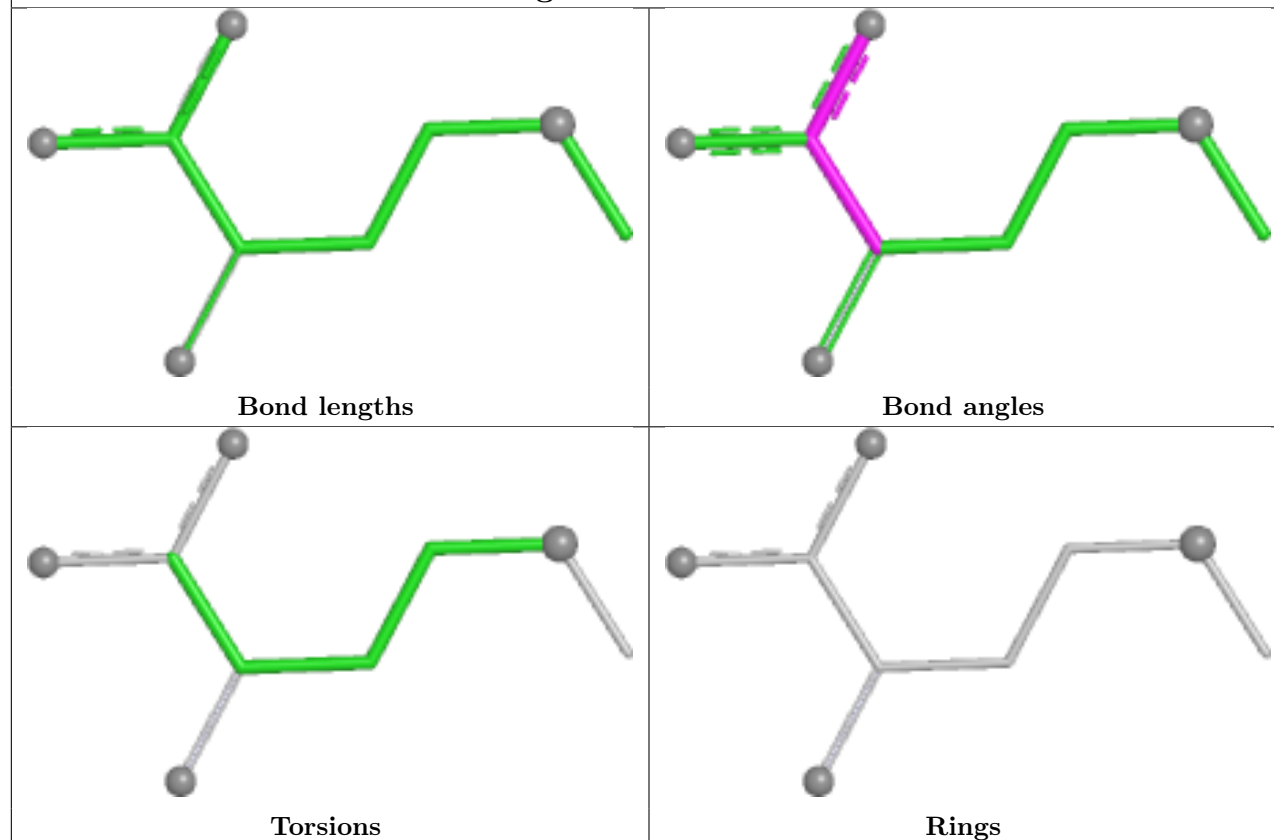
There are no ring outliers.

11 monomers are involved in 25 short contacts:

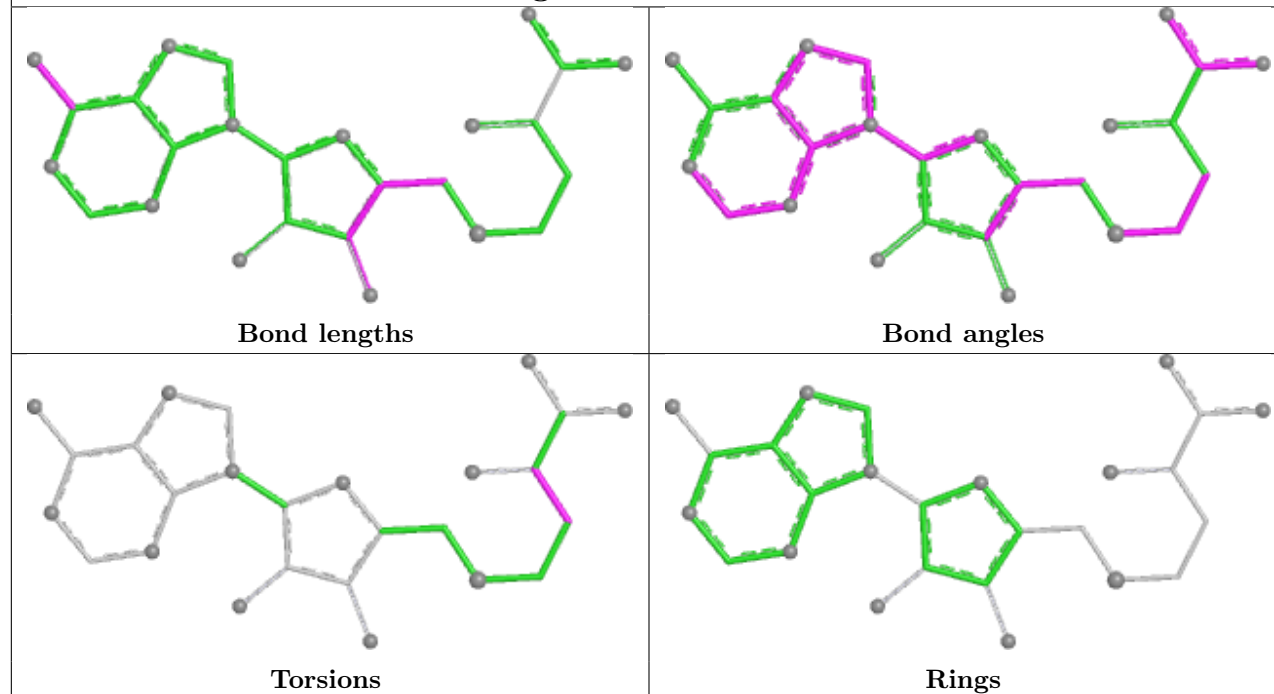
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	SAH	1	0
4	B	402	TRS	5	0
4	C	402	TRS	4	0
3	C	403	H9L	3	0
2	D	401	SAH	1	0
3	D	404	H9L	3	0
2	A	401	SAH	2	0
2	B	401	SAH	1	0
3	A	402	H9L	1	0
4	D	403	TRS	1	0
4	D	402	TRS	3	0

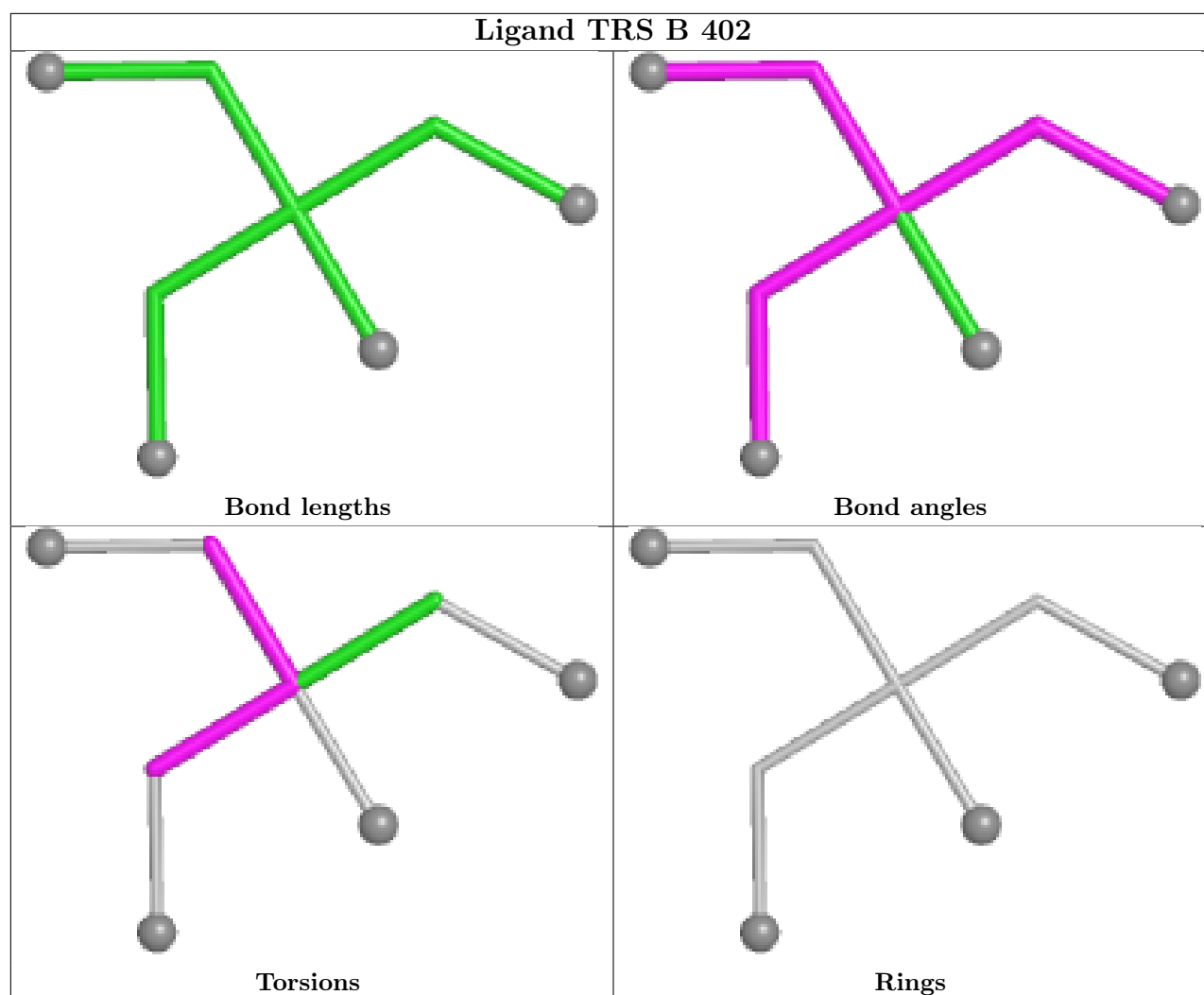
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

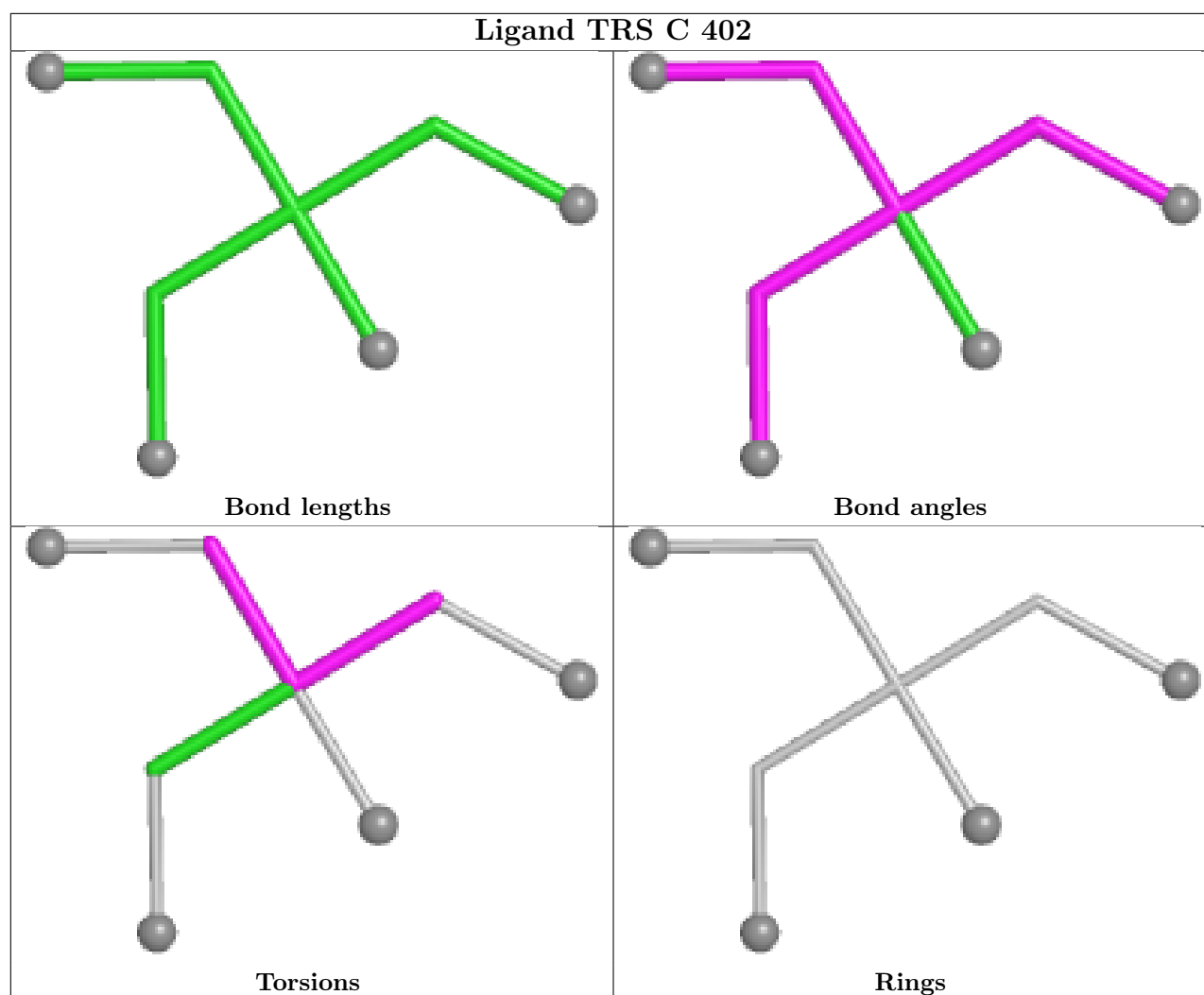
Ligand H9L B 403



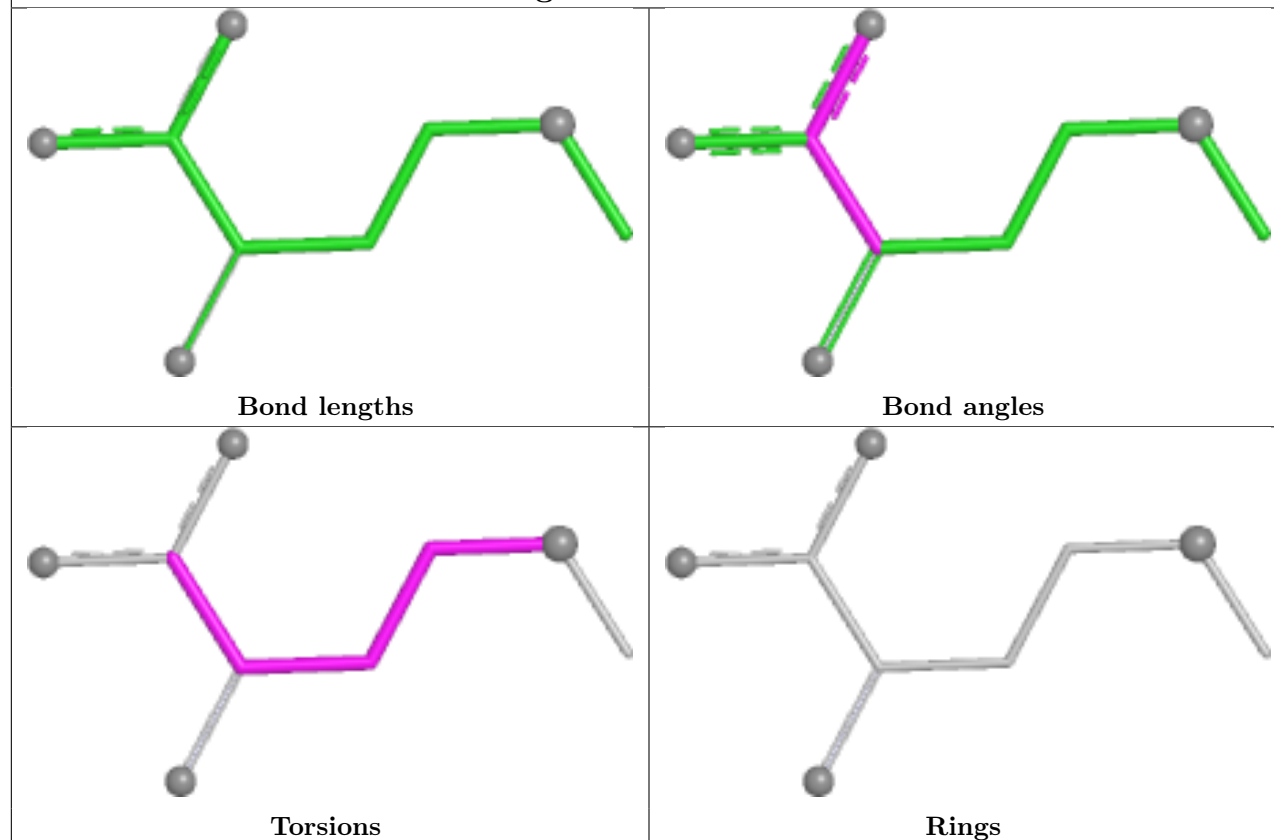
Ligand SAH C 401



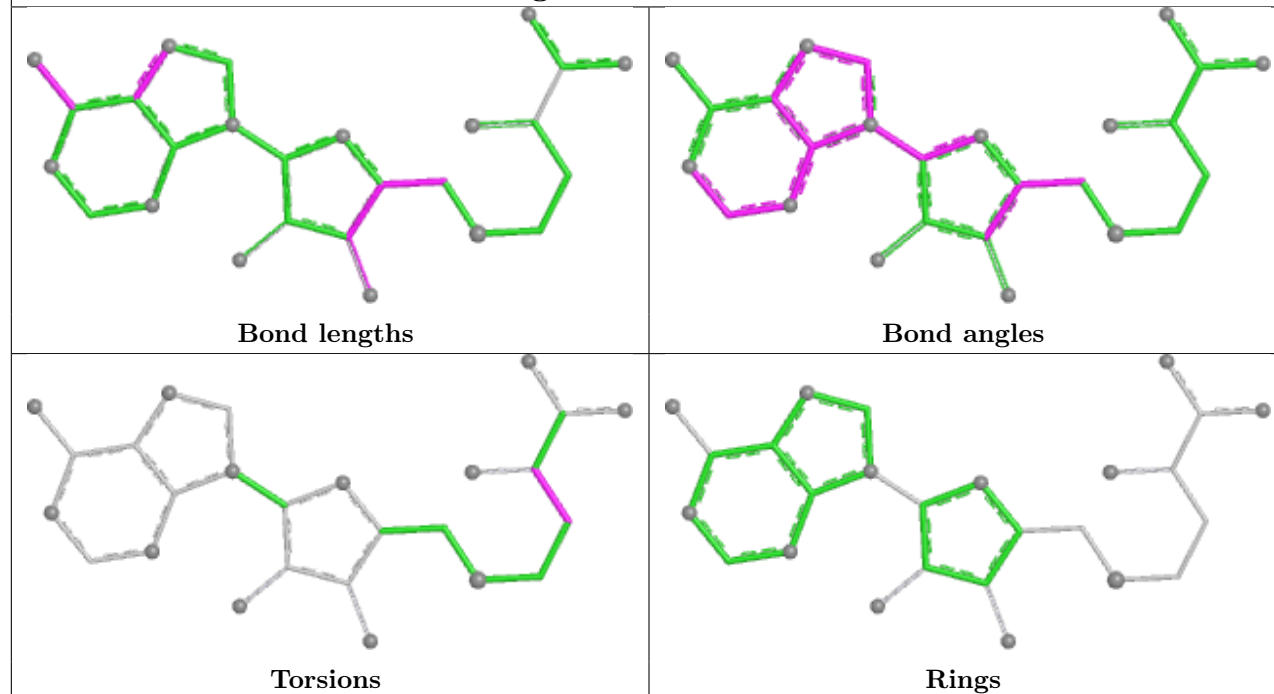




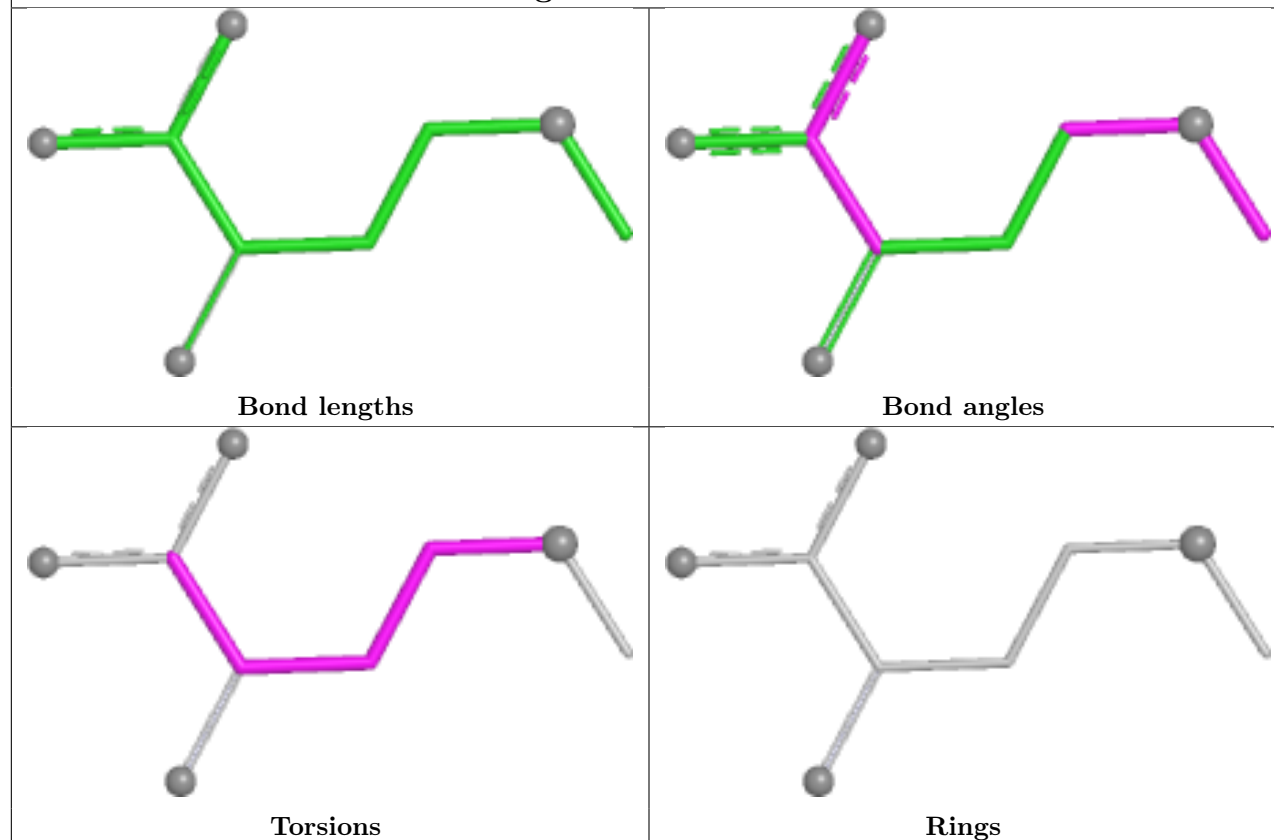
Ligand H9L C 403



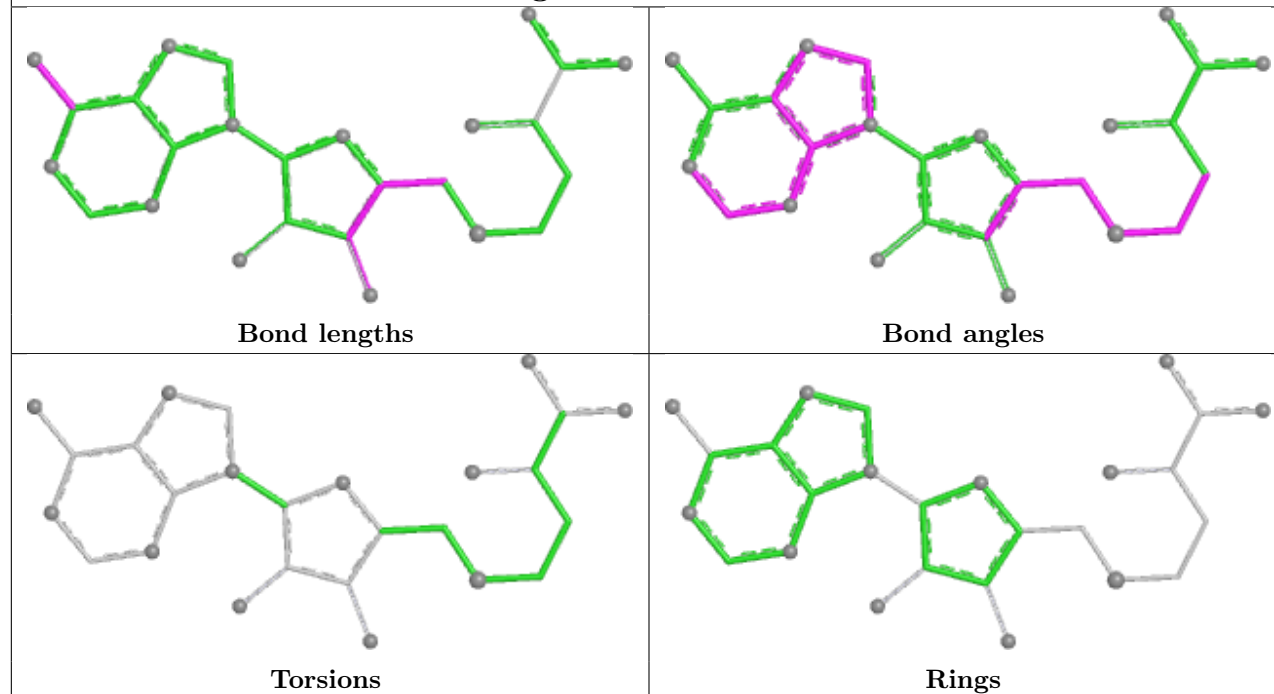
Ligand SAH D 401

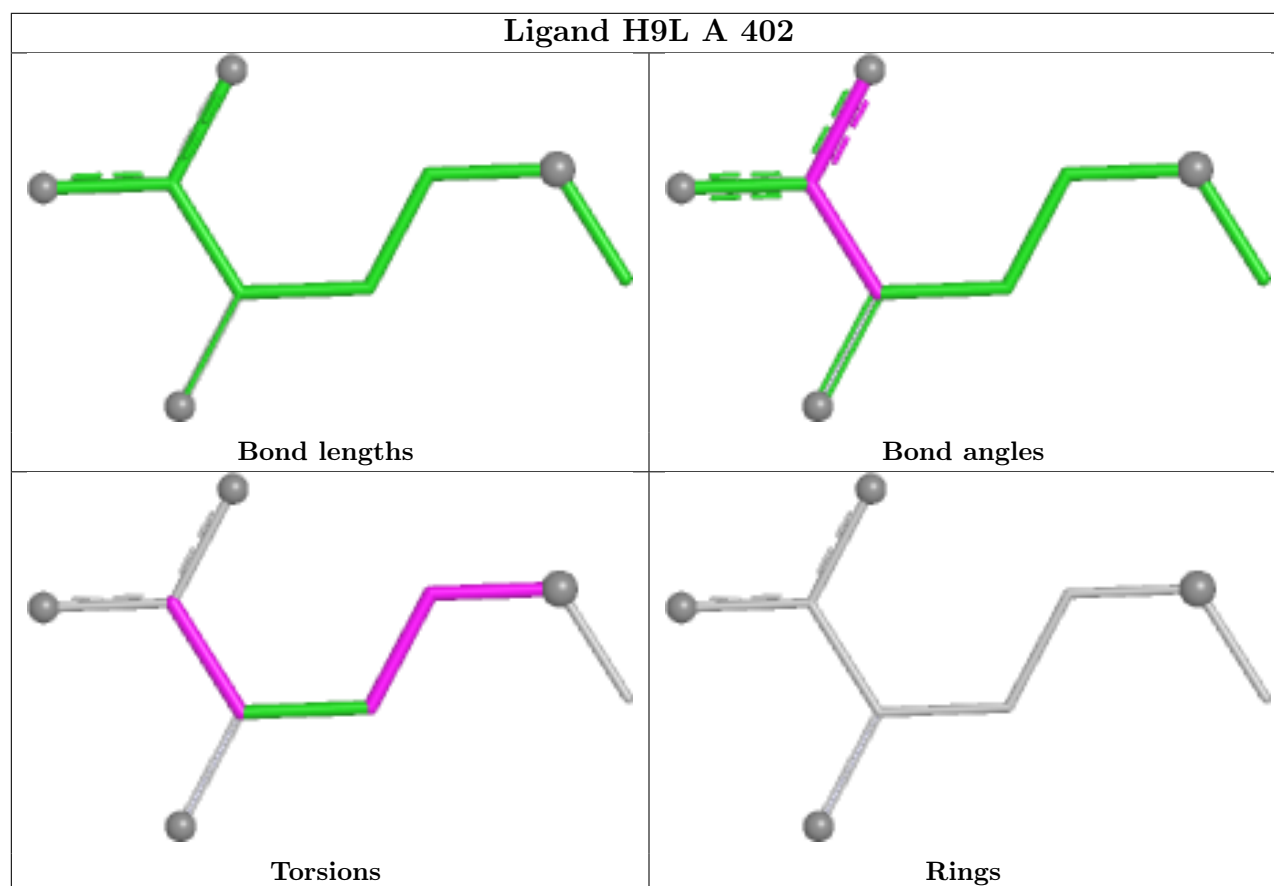
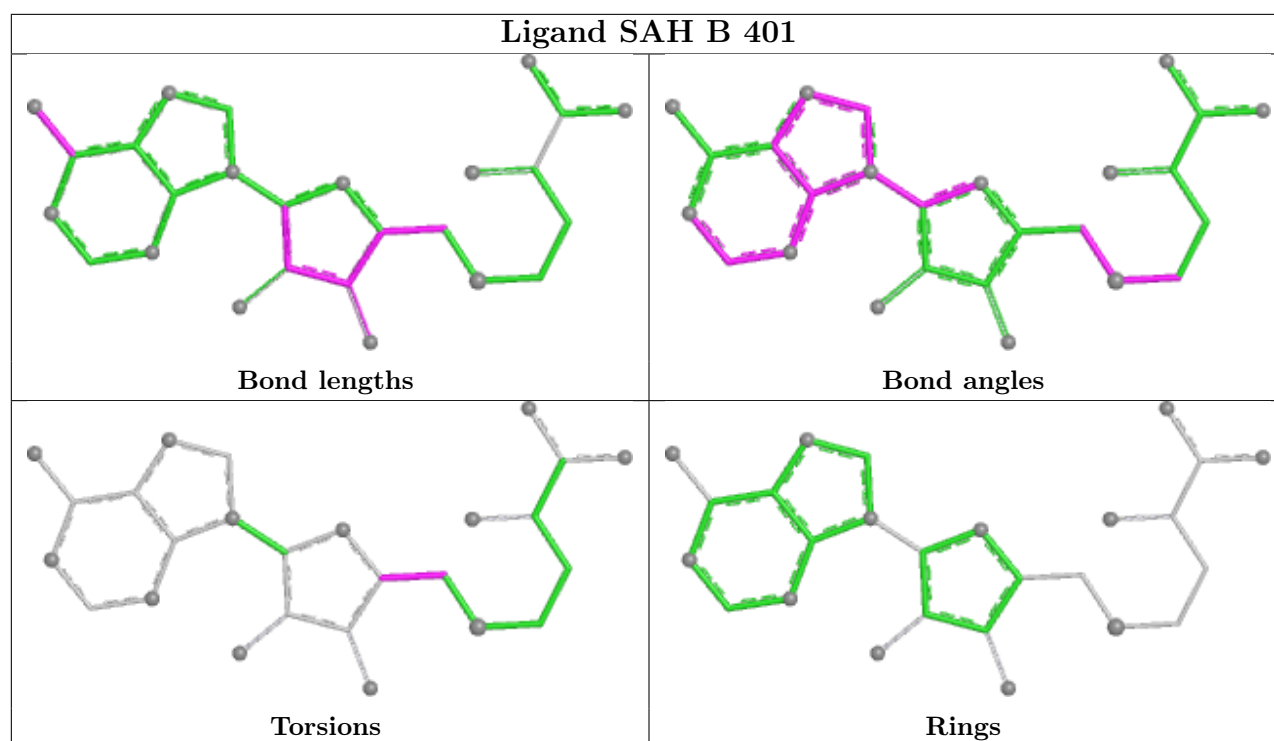


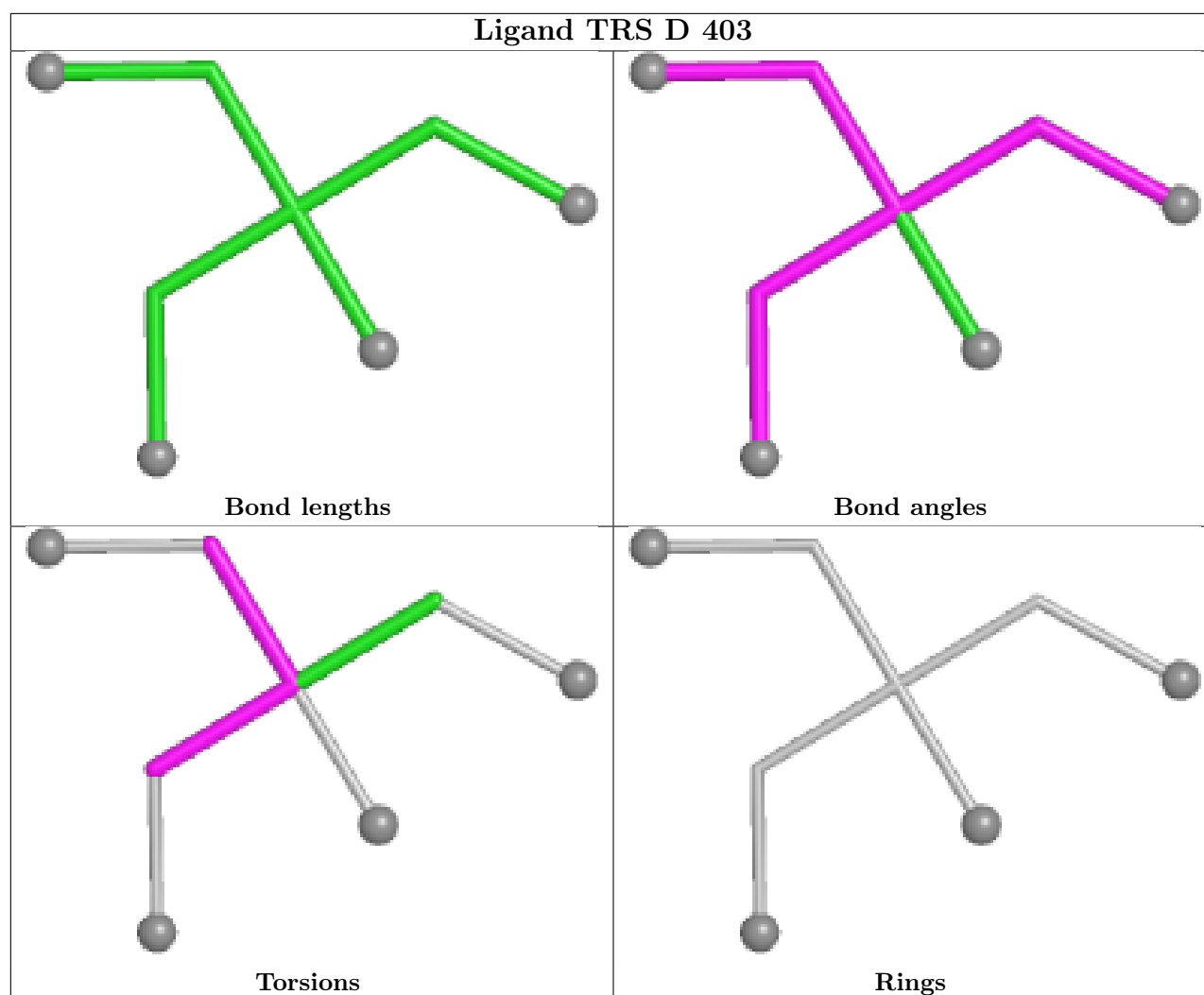
Ligand H9L D 404

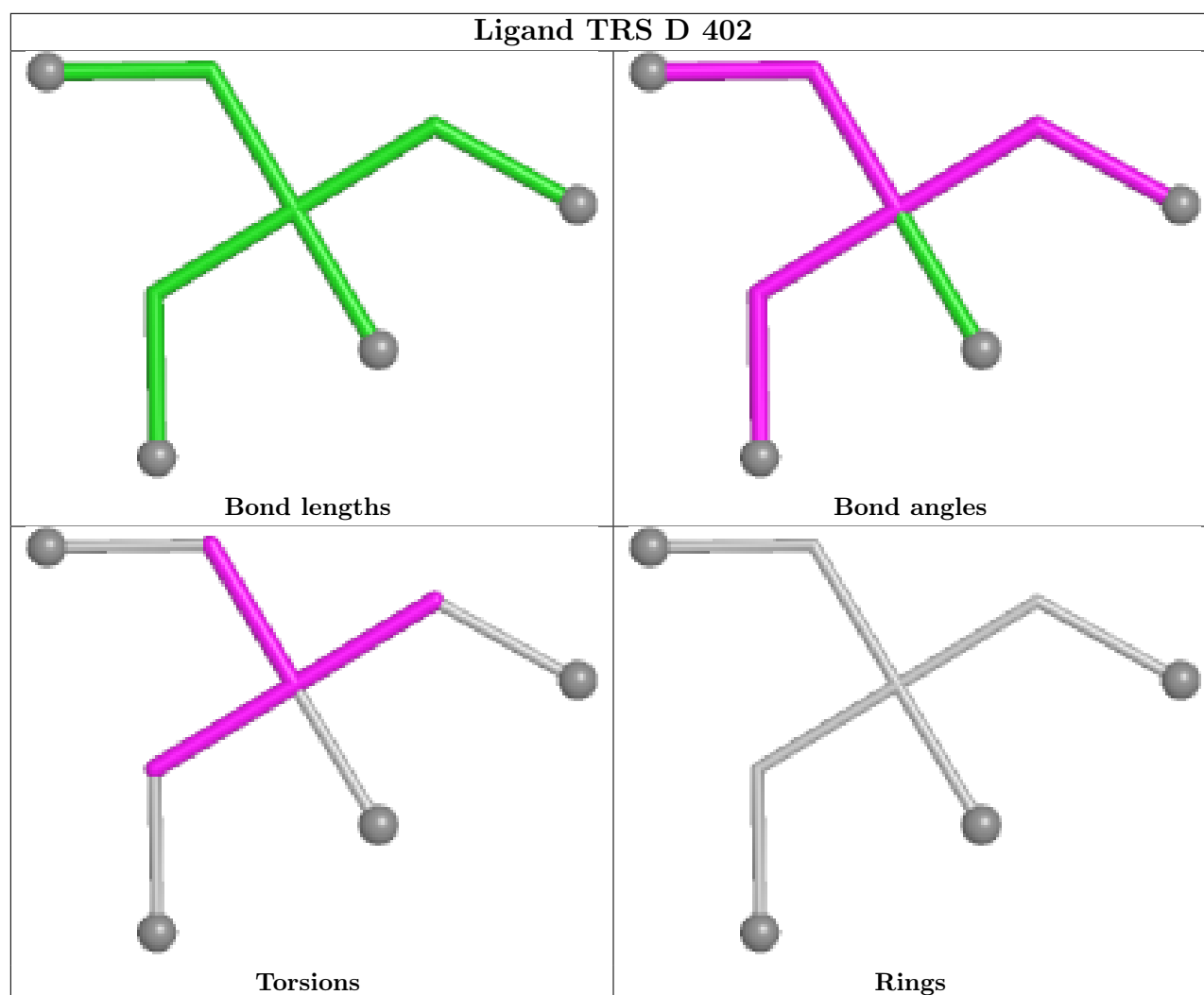


Ligand SAH A 401









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	336/343 (97%)	-0.09	0 100 100	26, 45, 62, 74	0
1	B	336/343 (97%)	-0.00	0 100 100	20, 45, 61, 75	2 (0%)
1	C	336/343 (97%)	-0.19	0 100 100	22, 40, 67, 76	3 (0%)
1	D	336/343 (97%)	-0.29	0 100 100	26, 37, 54, 80	0
All	All	1344/1372 (97%)	-0.14	0 100 100	20, 42, 60, 80	5 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
4	TRS	D	403	8/8	0.69	0.13	58,62,68,68	0
3	H9L	C	403	9/9	0.70	0.16	33,59,64,72	0
3	H9L	D	404	9/9	0.73	0.15	36,54,60,61	0
3	H9L	A	402	9/9	0.73	0.15	45,54,59,66	0

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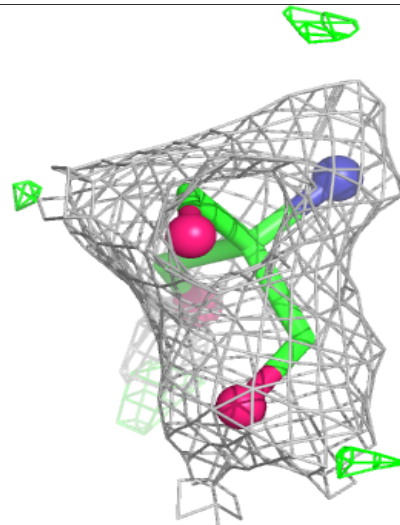
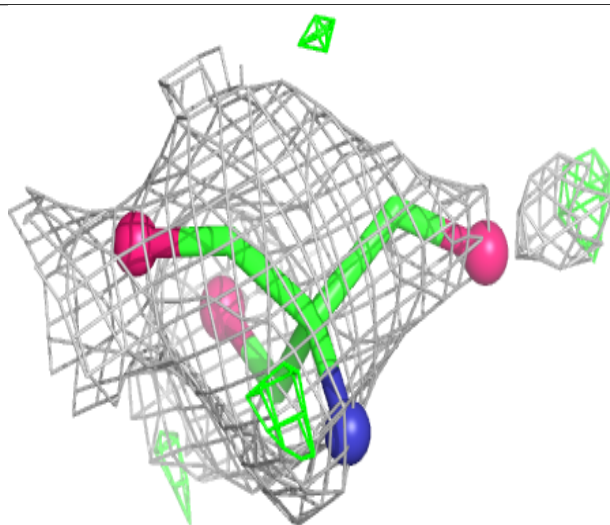
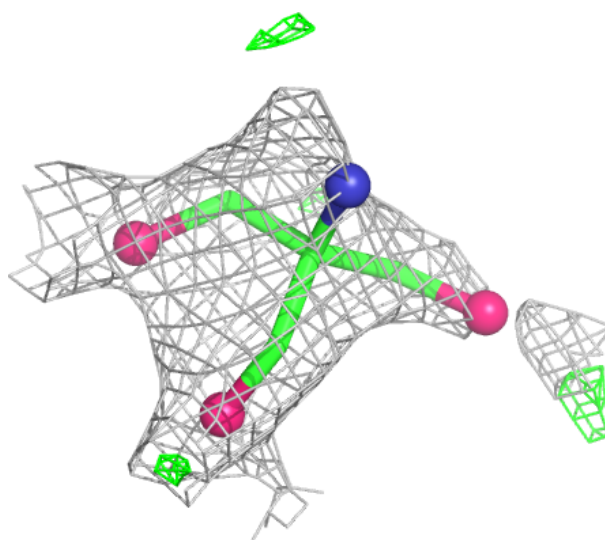
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	H9L	B	403	9/9	0.77	0.14	42,50,69,73	0
4	TRS	C	402	8/8	0.81	0.14	29,41,46,46	0
4	TRS	B	402	8/8	0.81	0.13	40,45,56,64	0
4	TRS	D	402	8/8	0.83	0.15	36,43,56,58	0
2	SAH	A	401	26/26	0.95	0.07	33,41,49,50	0
2	SAH	B	401	26/26	0.95	0.07	32,42,47,49	0
2	SAH	C	401	26/26	0.97	0.05	22,31,35,36	0
2	SAH	D	401	26/26	0.97	0.05	22,30,33,33	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.

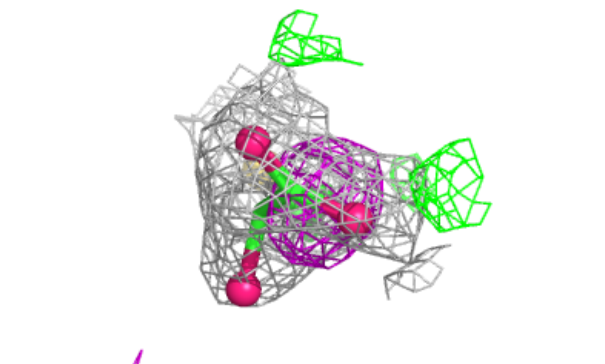
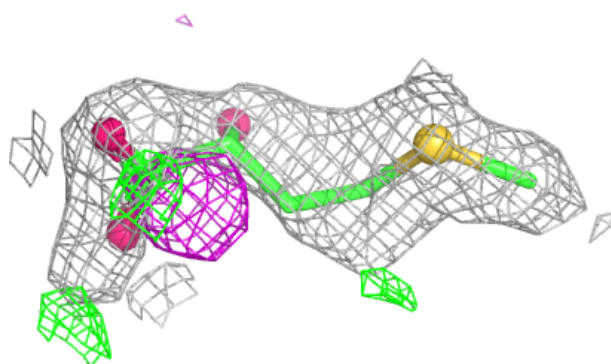
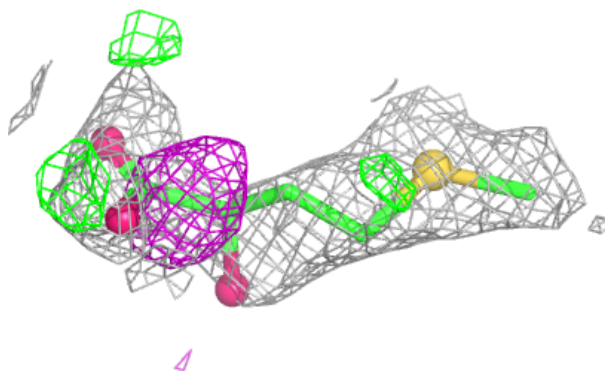
Electron density around TRS D 403:

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

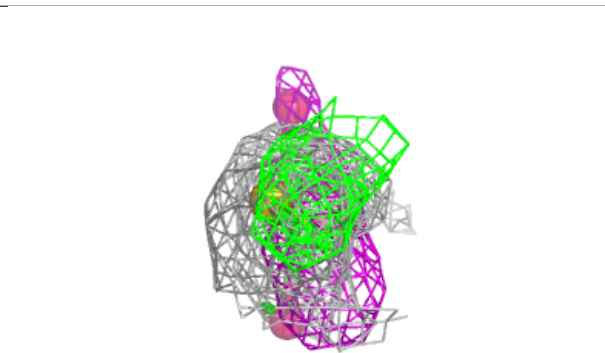
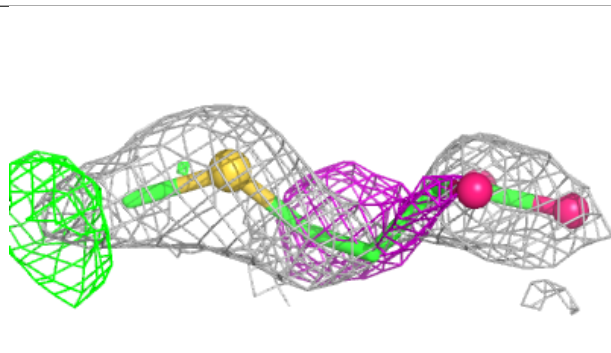
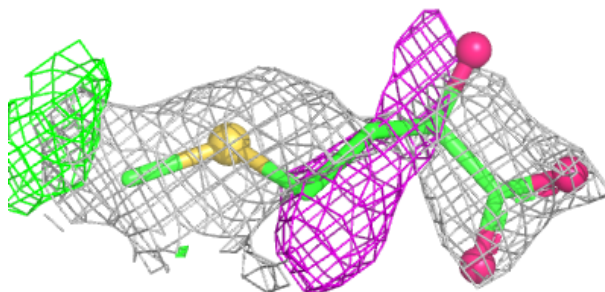


Electron density around H9L C 403:

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

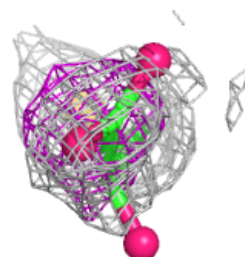
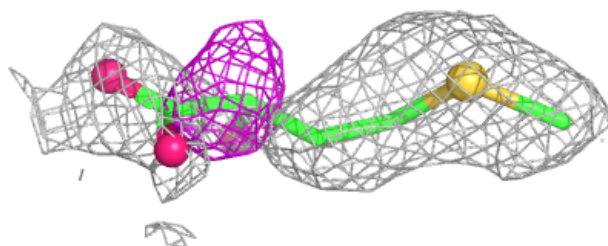
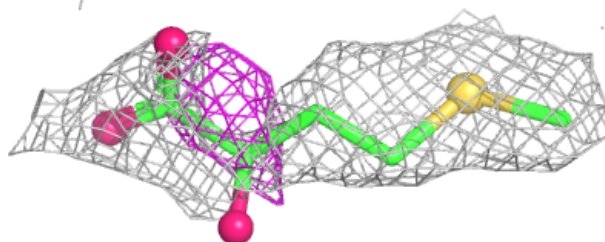
**Electron density around H9L D 404:**

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



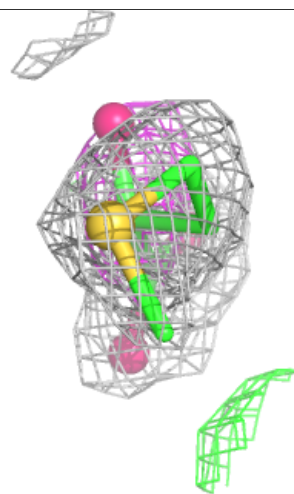
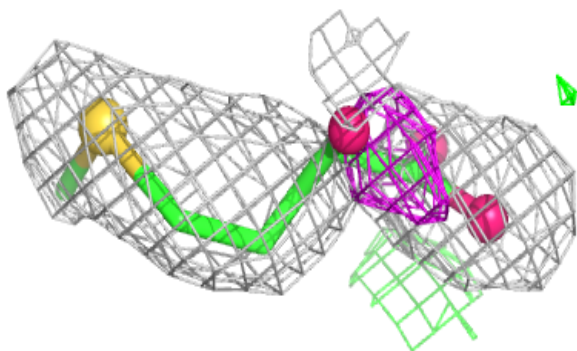
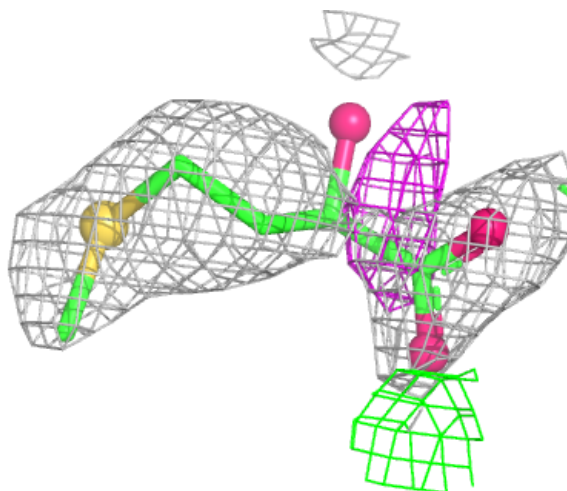
Electron density around H9L A 402:

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



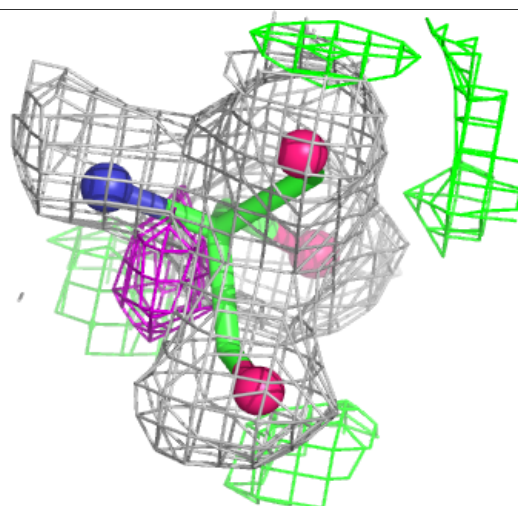
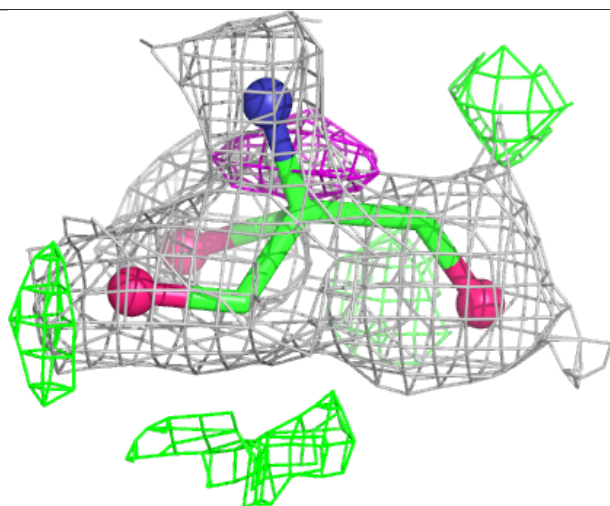
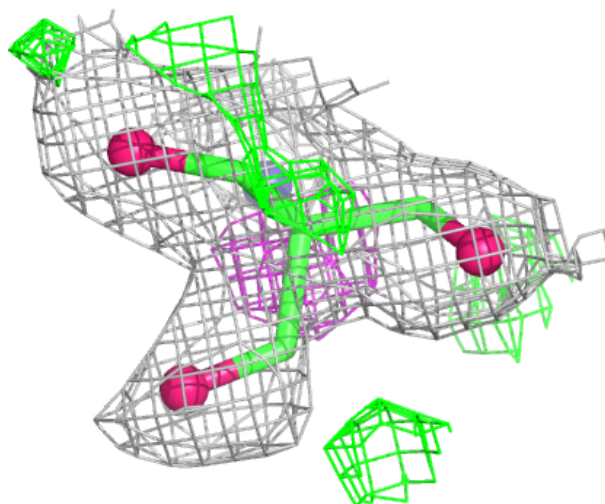
Electron density around H9L B 403:

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



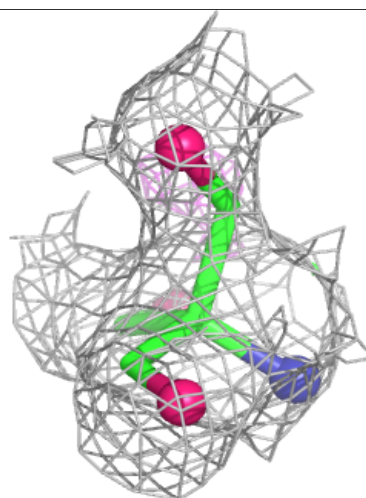
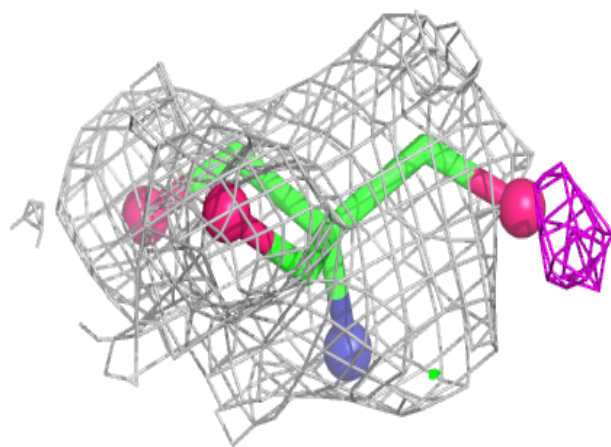
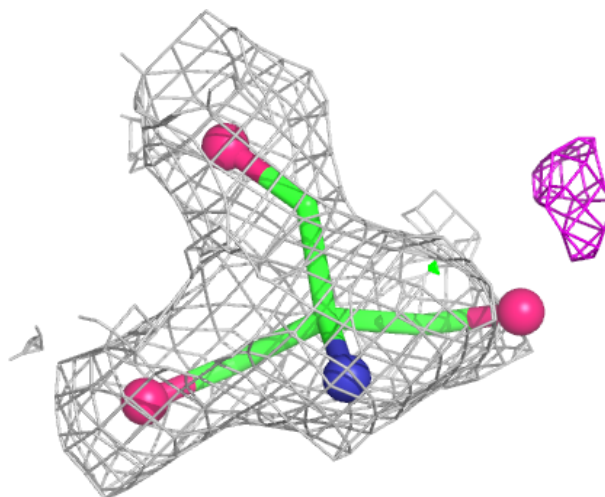
Electron density around TRS C 402:

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



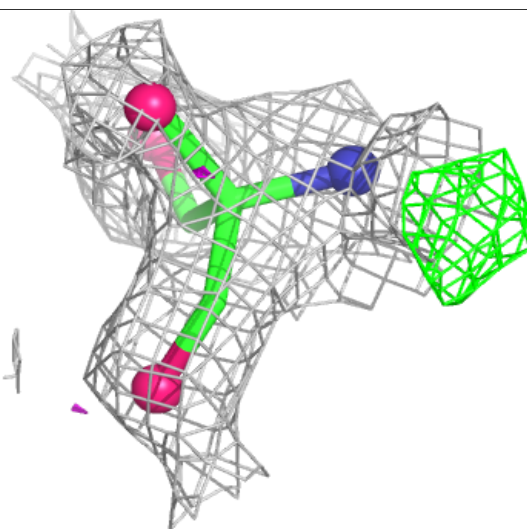
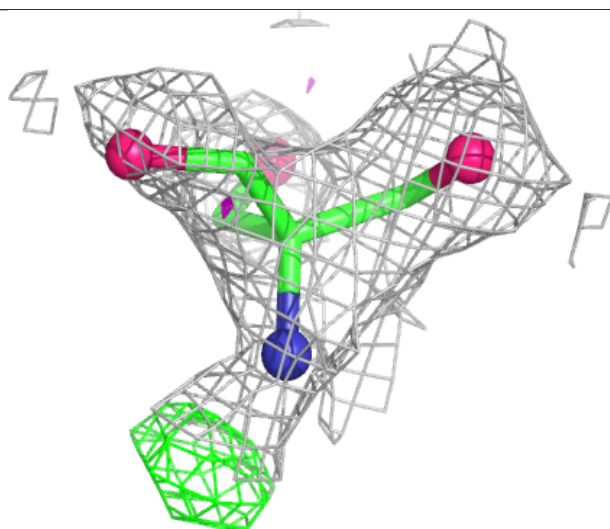
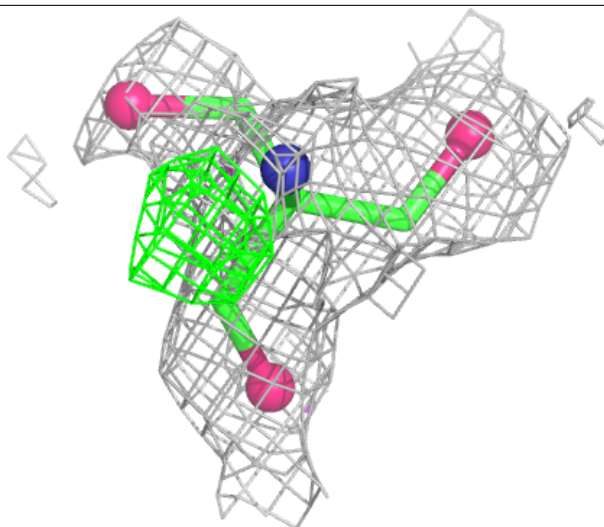
Electron density around TRS B 402:

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



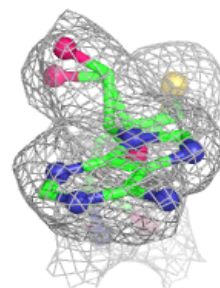
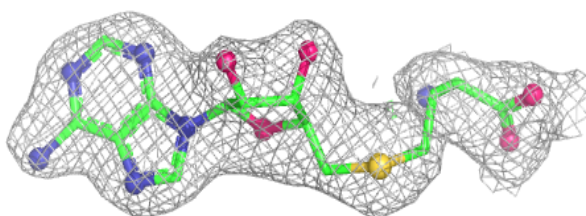
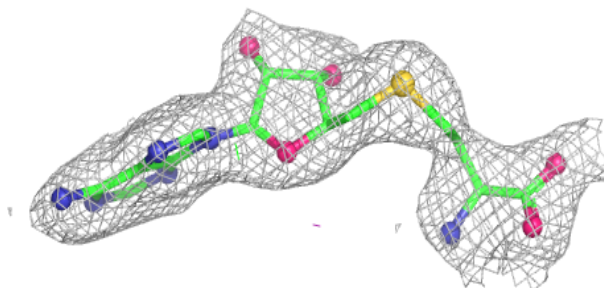
Electron density around TRS D 402:

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

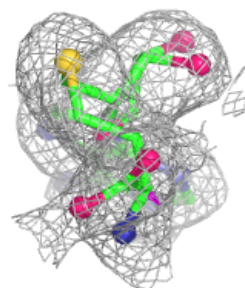
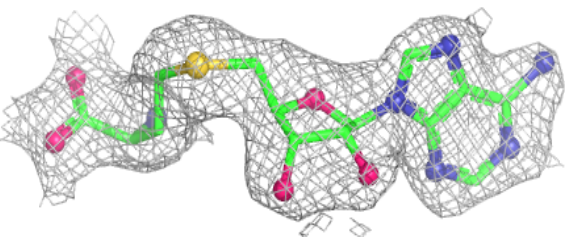
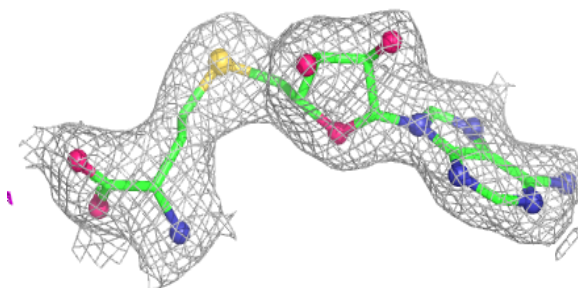


Electron density around SAH A 401:

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

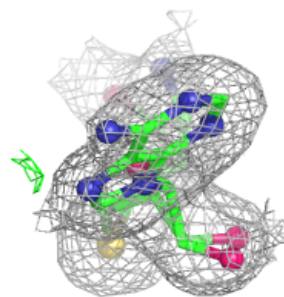
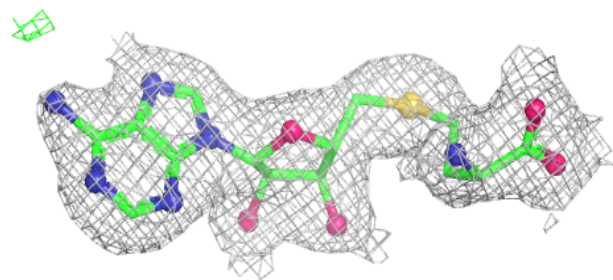
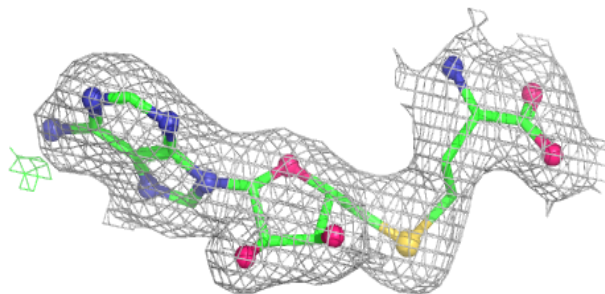
**Electron density around SAH B 401:**

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

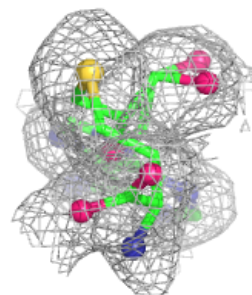
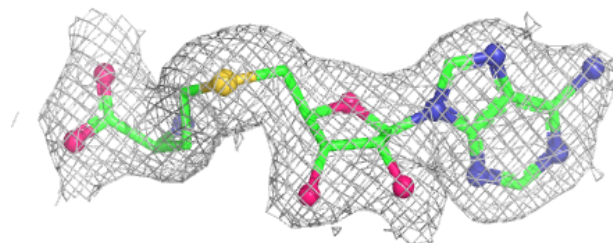
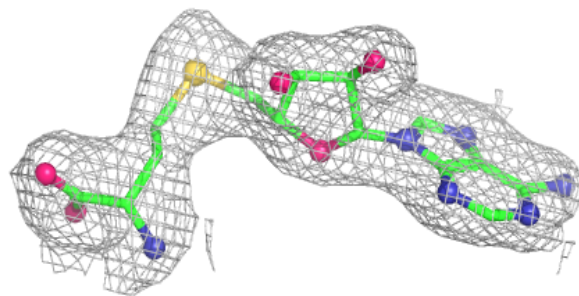


Electron density around SAH C 401:

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

**Electron density around SAH D 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.