



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 02:13 PM EDT

PDB ID : 9CBP / pdb_00009cbp
Title : Methionine synthase from *Thermus thermophilus* HB8, Homocysteine, Folate, and Cobalamin Domains, Pre-Catalytic State (Pre-Hcy-on)
Authors : Yamada, K.; Mendoza, J.; Koutmos, M.
Deposited on : 2024-06-19
Resolution : 2.45 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

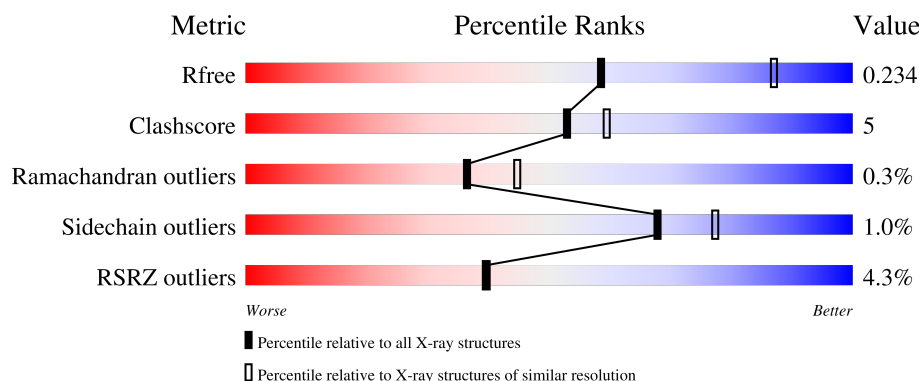
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	877	

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
5	GOL	A	911	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7037 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 Methionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	862	Total	C	N	O	S	0	1	0
			6634	4219	1163	1223	29			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	PHE	engineered mutation	UNP Q5SKM5
A	123	ALA	GLU	engineered mutation	UNP Q5SKM5
A	124	ALA	GLU	engineered mutation	UNP Q5SKM5
A	296	ALA	TYR	engineered mutation	UNP Q5SKM5
A	651	ALA	ASP	engineered mutation	UNP Q5SKM5
A	652	ALA	PRO	engineered mutation	UNP Q5SKM5
A	653	ALA	GLY	engineered mutation	UNP Q5SKM5

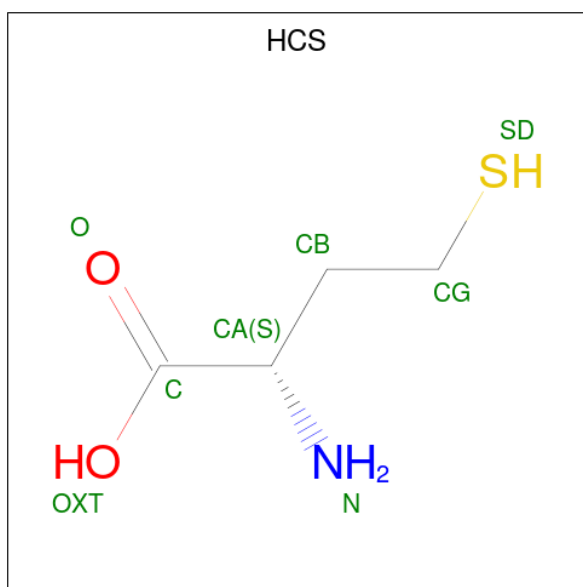
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

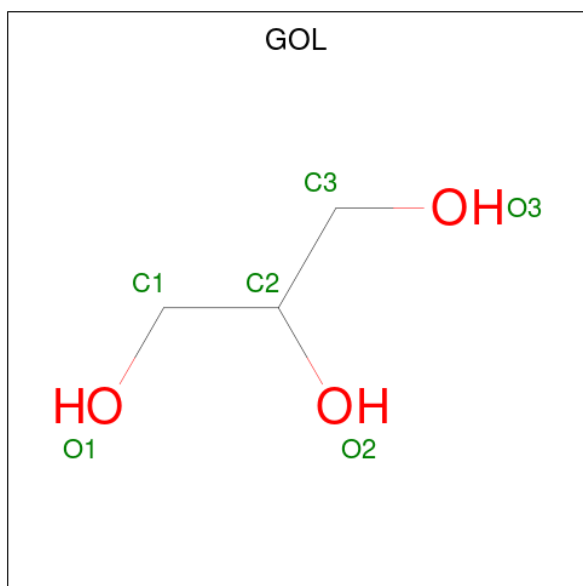
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		

- Molecule 4 is 2-AMINO-4-MERCAPTO-BUTYRIC ACID (CCD ID: HCS) (formula: C₄H₉NO₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			8	4	1	2	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



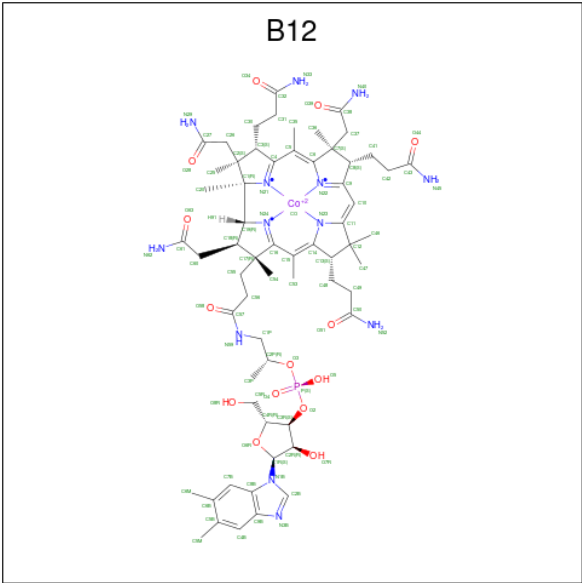
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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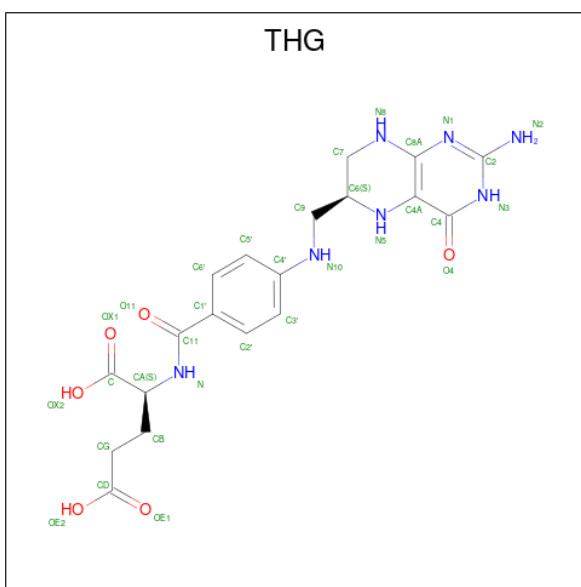
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is COBALAMIN (CCD ID: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P) (labeled as "Ligand of Interest" by depositor).



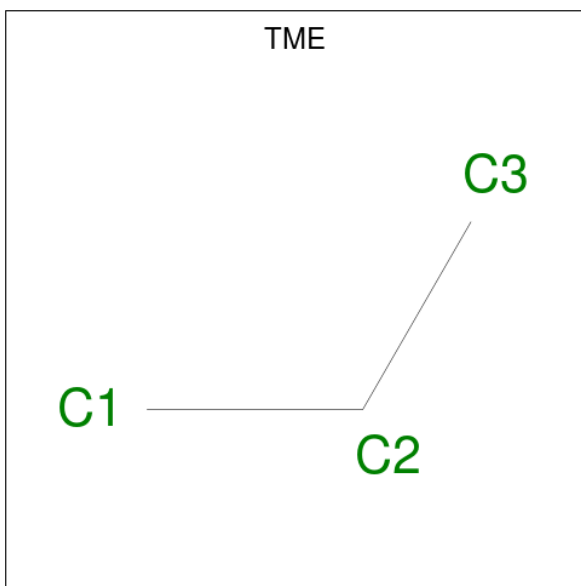
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 7 is (6S)-5,6,7,8-TETRAHYDROFOLATE (CCD ID: THG) (formula: C₁₉H₂₃N₇O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			32	19	7	6		

- Molecule 8 is PROPANE (CCD ID: TME) (formula: C₃H₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	C	0	0
			3	3		

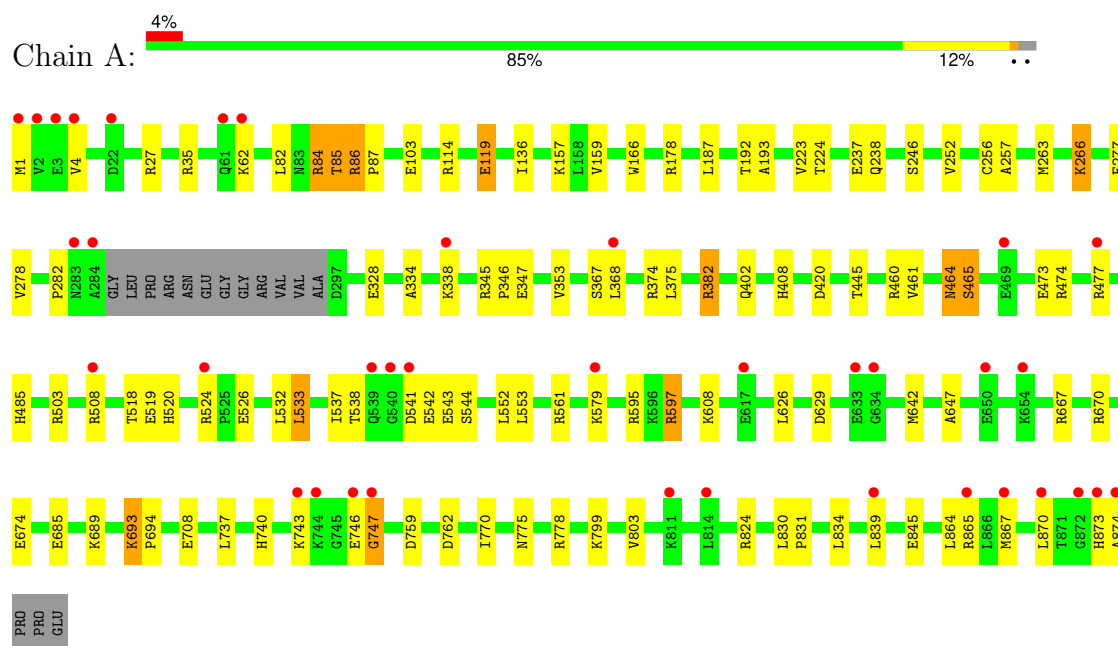
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	224	Total 224	O 224	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 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: Methionine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.95Å 83.82Å 163.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.99 – 2.45 81.86 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.1 (81.99-2.45) 98.4 (81.86-2.45)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0431	Depositor
R, R_{free}	0.161 , 0.233 0.178 , 0.234	Depositor DCC
R_{free} test set	1790 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7037	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TME, HCS, B12, GOL, K, ZN, THG

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	1.00	13/6754 (0.2%)	1.31	28/9139 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	17

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	LYS	C-N	13.51	1.51	1.33
1	A	474	ARG	C-N	9.89	1.46	1.33
1	A	473	GLU	C-N	-9.74	1.20	1.34
1	A	552	LEU	C-N	-7.95	1.23	1.33
1	A	553	LEU	C-N	7.63	1.43	1.33
1	A	346	PRO	C-N	-7.04	1.24	1.33
1	A	347	GLU	C-N	6.24	1.42	1.33
1	A	367	SER	C-N	6.10	1.41	1.33
1	A	740	HIS	CE1-NE2	-5.68	1.26	1.32
1	A	740	HIS	CG-CD2	-5.38	1.29	1.35
1	A	520	HIS	ND1-CE1	5.21	1.37	1.32
1	A	114	ARG	NE-CZ	5.14	1.38	1.33
1	A	485	HIS	CE1-NE2	-5.14	1.27	1.32

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	THR	CA-C-N	-9.57	98.44	121.80
1	A	85	THR	C-N-CA	-9.57	98.44	121.80
1	A	84	ARG	O-C-N	7.99	132.66	122.19
1	A	473	GLU	O-C-N	-7.80	113.66	122.09
1	A	62	LYS	CA-C-N	-7.75	109.97	120.90
1	A	62	LYS	C-N-CA	-7.75	109.97	120.90
1	A	693	LYS	CA-C-N	7.06	126.31	118.97
1	A	693	LYS	C-N-CA	7.06	126.31	118.97
1	A	524[A]	ARG	NE-CZ-NH2	-7.05	112.86	119.20
1	A	524[B]	ARG	NE-CZ-NH2	-7.05	112.86	119.20
1	A	552	LEU	O-C-N	-6.77	115.10	122.07
1	A	845	GLU	CB-CG-CD	6.28	123.27	112.60
1	A	346	PRO	O-C-N	-6.09	115.26	122.99
1	A	538	THR	CA-CB-OG1	-5.94	100.69	109.60
1	A	103	GLU	CG-CD-OE2	-5.93	104.77	118.40
1	A	445	THR	OG1-CB-CG2	-5.78	97.73	109.30
1	A	674	GLU	CB-CG-CD	5.59	122.11	112.60
1	A	519	GLU	CG-CD-OE2	5.52	131.09	118.40
1	A	461	VAL	N-CA-CB	-5.43	102.26	111.23
1	A	84	ARG	CD-NE-CZ	5.24	131.74	124.40
1	A	464	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	A	642	MET	CG-SD-CE	-5.22	89.42	100.90
1	A	526	GLU	CB-CG-CD	5.21	121.46	112.60
1	A	420	ASP	CA-C-N	5.12	127.09	120.44
1	A	420	ASP	C-N-CA	5.12	127.09	120.44
1	A	347	GLU	CA-C-N	-5.06	114.31	122.81
1	A	347	GLU	C-N-CA	-5.06	114.31	122.81
1	A	367	SER	O-C-N	5.04	128.99	123.25

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	ARG	Sidechain
1	A	35	ARG	Sidechain
1	A	374	ARG	Sidechain
1	A	382	ARG	Sidechain
1	A	464	ASN	Peptide
1	A	465	SER	Peptide
1	A	477	ARG	Sidechain
1	A	508	ARG	Sidechain
1	A	561	ARG	Sidechain
1	A	595	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	597	ARG	Sidechain
1	A	667	ARG	Sidechain
1	A	778	ARG	Sidechain
1	A	824	ARG	Sidechain
1	A	84	ARG	Sidechain
1	A	86	ARG	Sidechain
1	A	865	ARG	Sidechain

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	6634	0	6756	56	1
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	8	0	7	0	0
5	A	42	0	56	8	0
6	A	91	0	88	13	0
7	A	32	0	21	1	1
8	A	3	0	8	2	0
9	A	224	0	0	8	0
All	All	7037	0	6936	68	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (68) 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:334:ALA:O	1:A:338:LYS:HG3	1.65	0.95
5:A:908:GOL:H32	9:A:1003:HOH:O	1.81	0.79
6:A:910:B12:H552	6:A:910:B12:H531	1.68	0.74
1:A:166:TRP:HB3	5:A:907:GOL:H32	1.72	0.71
1:A:159:VAL:HG22	5:A:908:GOL:H31	1.72	0.70
1:A:503:ARG:HD3	9:A:1194:HOH:O	1.91	0.69
1:A:626:LEU:HD12	5:A:911:GOL:H32	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:HIS:HE2	6:A:910:B12:H402	1.48	0.62
1:A:1:MET:HG2	1:A:4:VAL:HG13	1.82	0.61
6:A:910:B12:H351	6:A:910:B12:H362	1.82	0.60
1:A:759:ASP:HA	6:A:910:B12:H452	1.69	0.58
1:A:608:LYS:CE	9:A:1009:HOH:O	2.53	0.57
1:A:834:LEU:HB3	1:A:839:LEU:HD21	1.86	0.57
1:A:670:ARG:HD2	9:A:1121:HOH:O	2.05	0.56
1:A:87:PRO:HB3	1:A:136:ILE:HD11	1.87	0.56
1:A:27:ARG:HG3	1:A:518:THR:HB	1.88	0.54
1:A:775:ASN:HD22	1:A:864:LEU:HD22	1.73	0.53
1:A:746:GLU:O	1:A:747:GLY:C	2.53	0.52
1:A:192:THR:HA	1:A:224:THR:OG1	2.10	0.51
1:A:252:VAL:O	1:A:278:VAL:HA	2.10	0.50
1:A:626:LEU:HD12	5:A:911:GOL:C3	2.42	0.50
1:A:82:LEU:O	1:A:86:ARG:N	2.36	0.49
1:A:263:MET:HE1	1:A:282:PRO:HA	1.92	0.49
1:A:224:THR:CG2	1:A:257:ALA:HB2	2.42	0.49
6:A:910:B12:H562	6:A:910:B12:H621	1.78	0.49
1:A:537:ILE:HG22	1:A:544:SER:O	2.13	0.48
1:A:867:MET:HE2	1:A:867:MET:HA	1.95	0.48
1:A:670:ARG:NH2	1:A:708:GLU:OE2	2.48	0.47
1:A:82:LEU:HA	1:A:85:THR:OG1	2.15	0.47
1:A:775:ASN:HD22	1:A:864:LEU:CD2	2.27	0.47
1:A:353:VAL:HG12	1:A:460:ARG:HG2	1.97	0.47
1:A:685:GLU:HG3	1:A:689:LYS:HE3	1.97	0.47
1:A:762:ASP:H	6:A:910:B12:H522	1.62	0.47
1:A:246:SER:HB2	9:A:1070:HOH:O	2.16	0.46
1:A:503:ARG:HB2	9:A:1194:HOH:O	2.16	0.46
1:A:532:LEU:O	1:A:533:LEU:HB2	2.14	0.46
1:A:237:GLU:HG2	1:A:238:GLN:N	2.30	0.46
6:A:910:B12:H621	6:A:910:B12:H18	1.58	0.46
1:A:579:LYS:HE3	1:A:579:LYS:HB2	1.66	0.45
1:A:693:LYS:HA	1:A:693:LYS:HD3	1.78	0.45
1:A:803:VAL:HG23	1:A:830:LEU:HD23	1.97	0.45
1:A:694:PRO:HB3	1:A:737:LEU:HB3	1.97	0.45
1:A:831:PRO:HG2	1:A:870:LEU:HD12	1.99	0.45
7:A:912:THG:HN	7:A:912:THG:HCG1	1.55	0.45
1:A:629:ASP:HA	5:A:911:GOL:O3	2.17	0.44
1:A:157:LYS:HA	1:A:157:LYS:HD3	1.81	0.44
6:A:910:B12:H481	6:A:910:B12:H473	1.81	0.44
1:A:647:ALA:C	9:A:1001:HOH:O	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:LYS:HE3	1:A:743:LYS:HB3	1.81	0.43
1:A:375:LEU:HG	1:A:402:GLN:HE22	1.83	0.43
1:A:159:VAL:O	5:A:908:GOL:H12	2.19	0.43
1:A:328:GLU:H	1:A:328:GLU:CD	2.26	0.43
6:A:910:B12:H262	6:A:910:B12:H91	1.79	0.42
6:A:910:B12:C16	8:A:914:TME:H32	2.50	0.42
1:A:537:ILE:HB	5:A:911:GOL:H12	2.02	0.42
1:A:775:ASN:ND2	1:A:864:LEU:HD22	2.34	0.42
1:A:542:GLU:O	1:A:542:GLU:HG3	2.18	0.42
6:A:910:B12:O2	6:A:910:B12:H2B	2.20	0.42
1:A:193:ALA:HB3	1:A:223:VAL:HA	2.01	0.41
6:A:910:B12:H362	6:A:910:B12:C35	2.50	0.41
1:A:597:ARG:HD3	1:A:597:ARG:HA	1.75	0.41
1:A:266:LYS:H	1:A:266:LYS:HG2	1.61	0.41
1:A:382:ARG:HA	1:A:382:ARG:HD2	1.78	0.41
1:A:873:HIS:O	1:A:874:ALA:C	2.63	0.41
6:A:910:B12:C14	8:A:914:TME:H32	2.50	0.41
1:A:277:PHE:HA	1:A:345:ARG:HD2	2.04	0.40
1:A:541:ASP:OD1	1:A:541:ASP:N	2.52	0.40
1:A:799:LYS:HA	9:A:1065:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:OE1	7:A:912:THG:OX2[4_555]	2.10	0.10

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	859/877 (98%)	832 (97%)	24 (3%)	3 (0%)	36	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	SER
1	A	747	GLY
1	A	533	LEU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	680/690 (99%)	673 (99%)	7 (1%)	68 77

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	GLU
1	A	187	LEU
1	A	256	CYS
1	A	266	LYS
1	A	368	LEU
1	A	543	GLU
1	A	770	ILE

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

Mol	Chain	Res	Type
1	A	352	GLN
1	A	402	GLN
1	A	774	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	A	909	-	5,5,5	0.33	0	5,5,5	0.60	0
5	GOL	A	908	-	5,5,5	0.31	0	5,5,5	0.83	0
7	THG	A	912	-	32,34,34	0.73	1 (3%)	39,47,47	0.91	1 (2%)
5	GOL	A	907	-	5,5,5	0.35	0	5,5,5	0.91	0
5	GOL	A	906	-	5,5,5	0.58	0	5,5,5	0.63	0
5	GOL	A	904	-	5,5,5	0.09	0	5,5,5	0.32	0
5	GOL	A	905	-	5,5,5	0.22	0	5,5,5	0.55	0
5	GOL	A	911	-	5,5,5	0.24	0	5,5,5	0.61	0
6	B12	A	910	1	94,101,101	0.55	2 (2%)	149,166,166	0.85	4 (2%)
8	TME	A	914	-	2,2,2	0.19	0	1,1,1	0.30	0
4	HCS	A	903	2	6,7,7	1.56	1 (16%)	5,8,8	0.86	0

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
5	GOL	A	909	-	-	2/4/4/4	-
5	GOL	A	908	-	-	3/4/4/4	-
7	THG	A	912	-	-	11/22/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	907	-	-	0/4/4/4	-
5	GOL	A	906	-	-	4/4/4/4	-
5	GOL	A	904	-	-	2/4/4/4	-
5	GOL	A	905	-	-	1/4/4/4	-
5	GOL	A	911	-	-	1/4/4/4	-
6	B12	A	910	1	-	19/56/223/223	0/3/11/11
4	HCS	A	903	2	-	3/7/7/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	HCS	O-C	3.50	1.32	1.22
6	A	910	B12	C16-C15	-2.26	1.38	1.44
7	A	912	THG	C4A-C8A	2.17	1.42	1.38
6	A	910	B12	C9-N22	2.04	1.35	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	912	THG	C2-N1-C8A	3.07	118.77	113.36
6	A	910	B12	C19-N24-C16	2.98	110.55	107.29
6	A	910	B12	C9-N22-C6	2.89	108.75	105.28
6	A	910	B12	C9B-C8B-N1B	2.15	106.26	105.30
6	A	910	B12	C19-C1-N21	2.10	104.30	102.14

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	903	HCS	N-CA-CB-CG
4	A	903	HCS	C-CA-CB-CG
5	A	904	GOL	C1-C2-C3-O3
5	A	908	GOL	O2-C2-C3-O3
5	A	909	GOL	C1-C2-C3-O3
6	A	910	B12	C3-C30-C31-C32
6	A	910	B12	C18-C60-C61-O63
6	A	910	B12	C18-C60-C61-N62
6	A	910	B12	C1P-C2P-O3-P
7	A	912	THG	N-CA-CB-CG
7	A	912	THG	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
5	A	906	GOL	O1-C1-C2-C3
5	A	906	GOL	C1-C2-C3-O3
5	A	908	GOL	O1-C1-C2-C3
5	A	908	GOL	C1-C2-C3-O3
5	A	904	GOL	O2-C2-C3-O3
5	A	905	GOL	O2-C2-C3-O3
7	A	912	THG	OX2-C-CA-N
7	A	912	THG	C1'-C11-N-CA
6	A	910	B12	C12-C13-C48-C49
6	A	910	B12	C14-C13-C48-C49
7	A	912	THG	OX1-C-CA-N
7	A	912	THG	O11-C11-N-CA
7	A	912	THG	CA-CB-CG-CD
6	A	910	B12	C18-C17-C55-C56
6	A	910	B12	O6R-C4R-C5R-O8R
6	A	910	B12	C41-C42-C43-O44
5	A	906	GOL	O1-C1-C2-O2
5	A	909	GOL	O2-C2-C3-O3
6	A	910	B12	C3P-C2P-O3-P
6	A	910	B12	C2R-C1R-N1B-C2B
6	A	910	B12	C41-C42-C43-N45
7	A	912	THG	C7-C6-C9-N10
6	A	910	B12	C2R-C1R-N1B-C8B
6	A	910	B12	O6R-C1R-N1B-C8B
5	A	906	GOL	O2-C2-C3-O3
7	A	912	THG	OE2-CD-CG-CB
6	A	910	B12	O6R-C1R-N1B-C2B
5	A	911	GOL	O1-C1-C2-C3
6	A	910	B12	C42-C41-C8-C9
7	A	912	THG	OE1-CD-CG-CB
6	A	910	B12	C16-C17-C55-C56
6	A	910	B12	C2P-O3-P-O4
6	A	910	B12	C2P-O3-P-O5
4	A	903	HCS	OXT-C-CA-N
7	A	912	THG	N5-C6-C9-N10

There are no ring outliers.

6 monomers are involved in 23 short contacts:

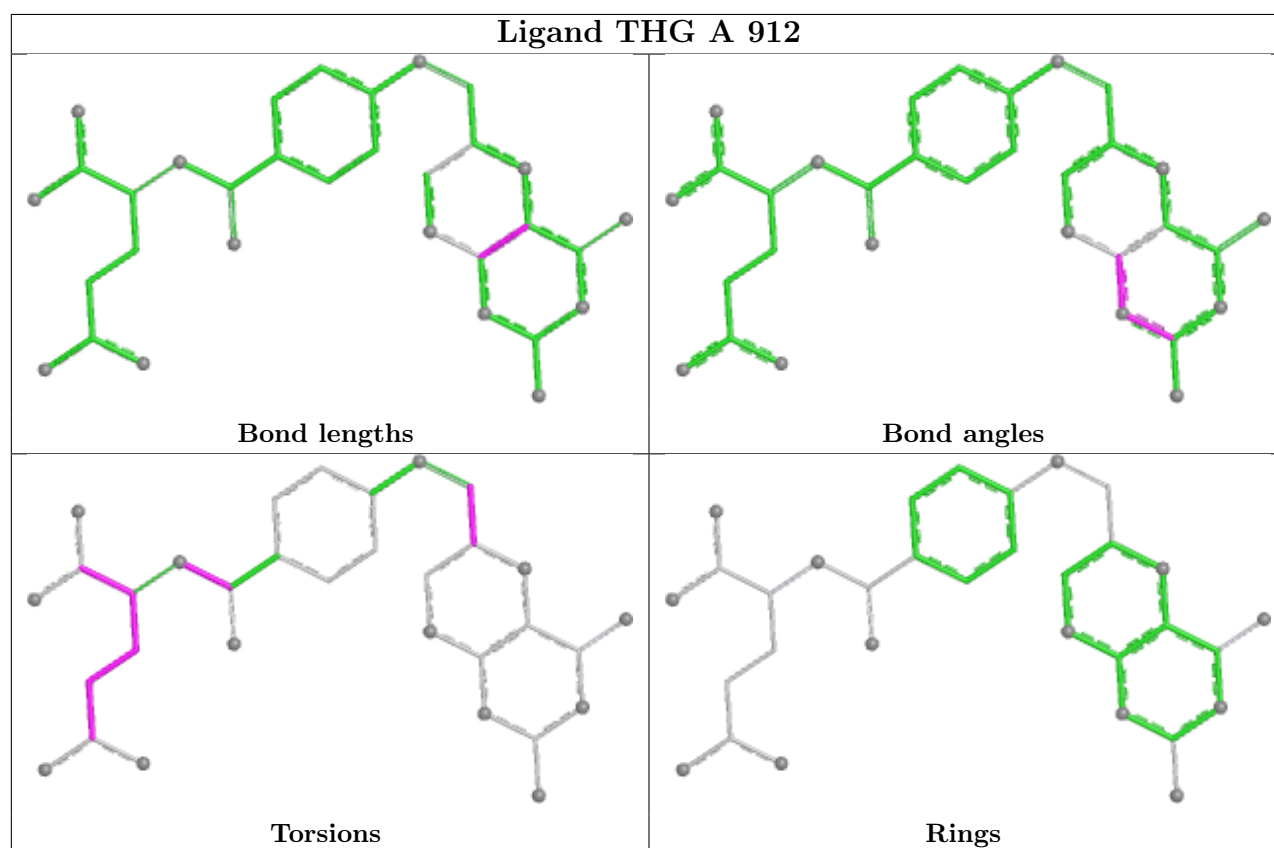
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	908	GOL	3	0
7	A	912	THG	1	1

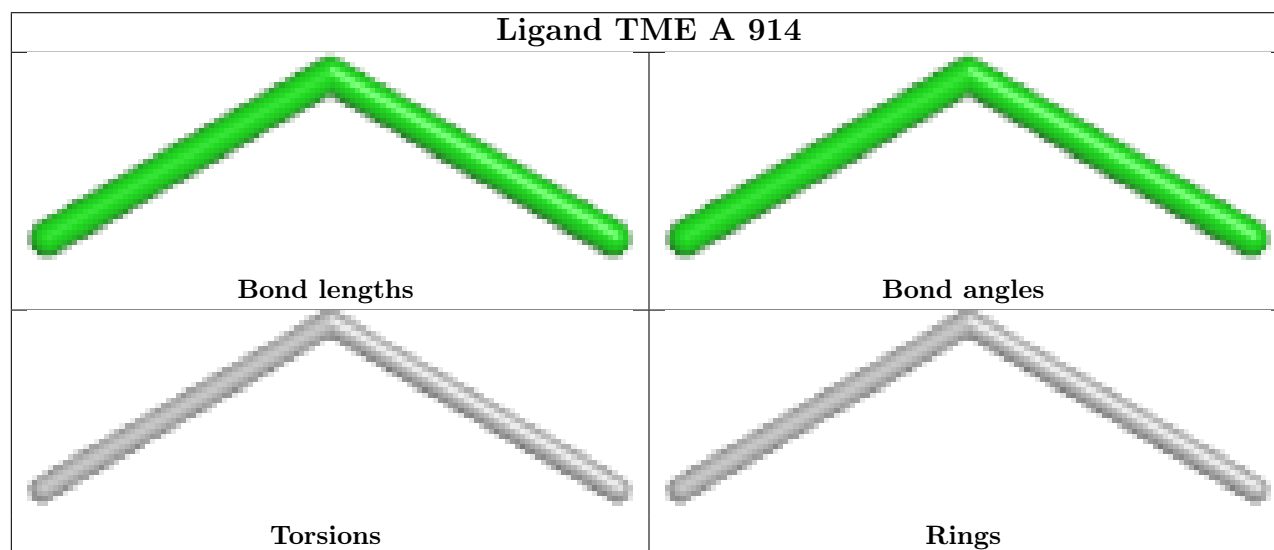
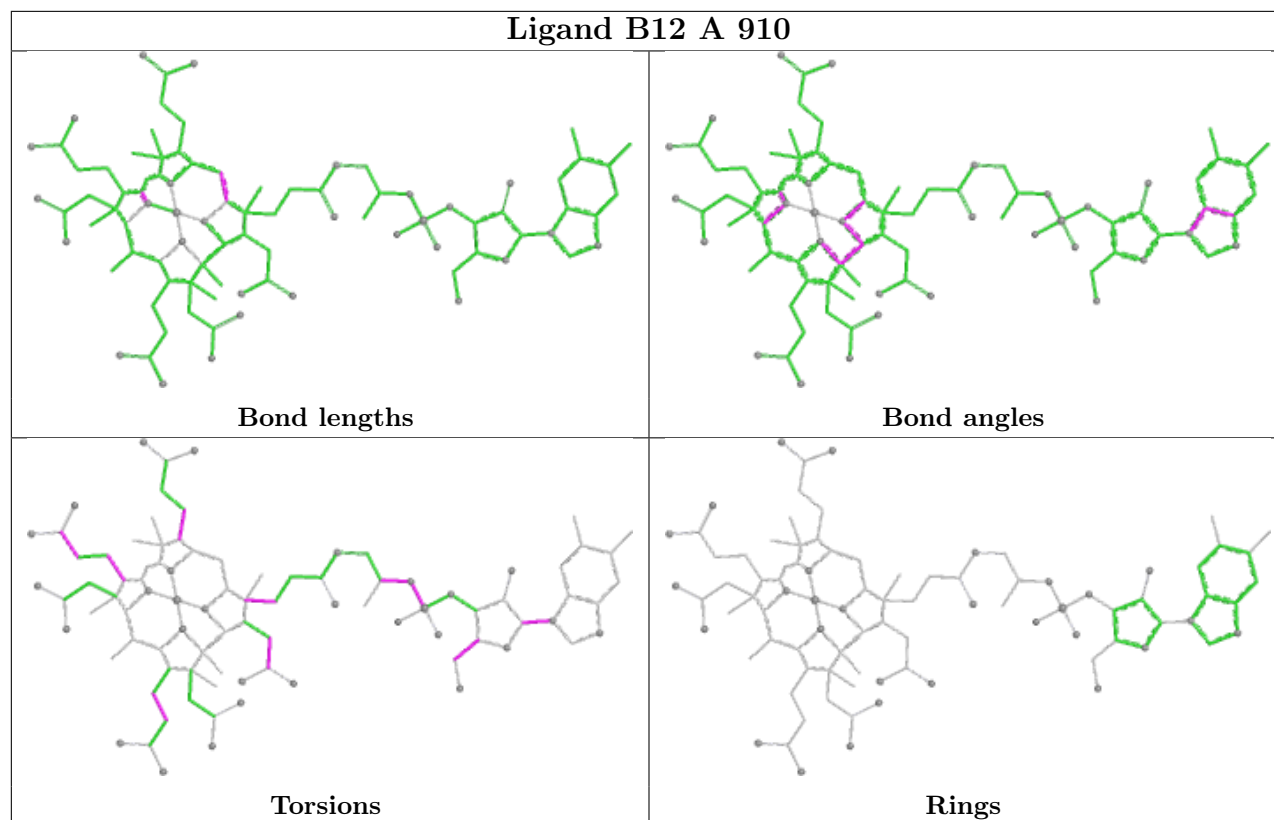
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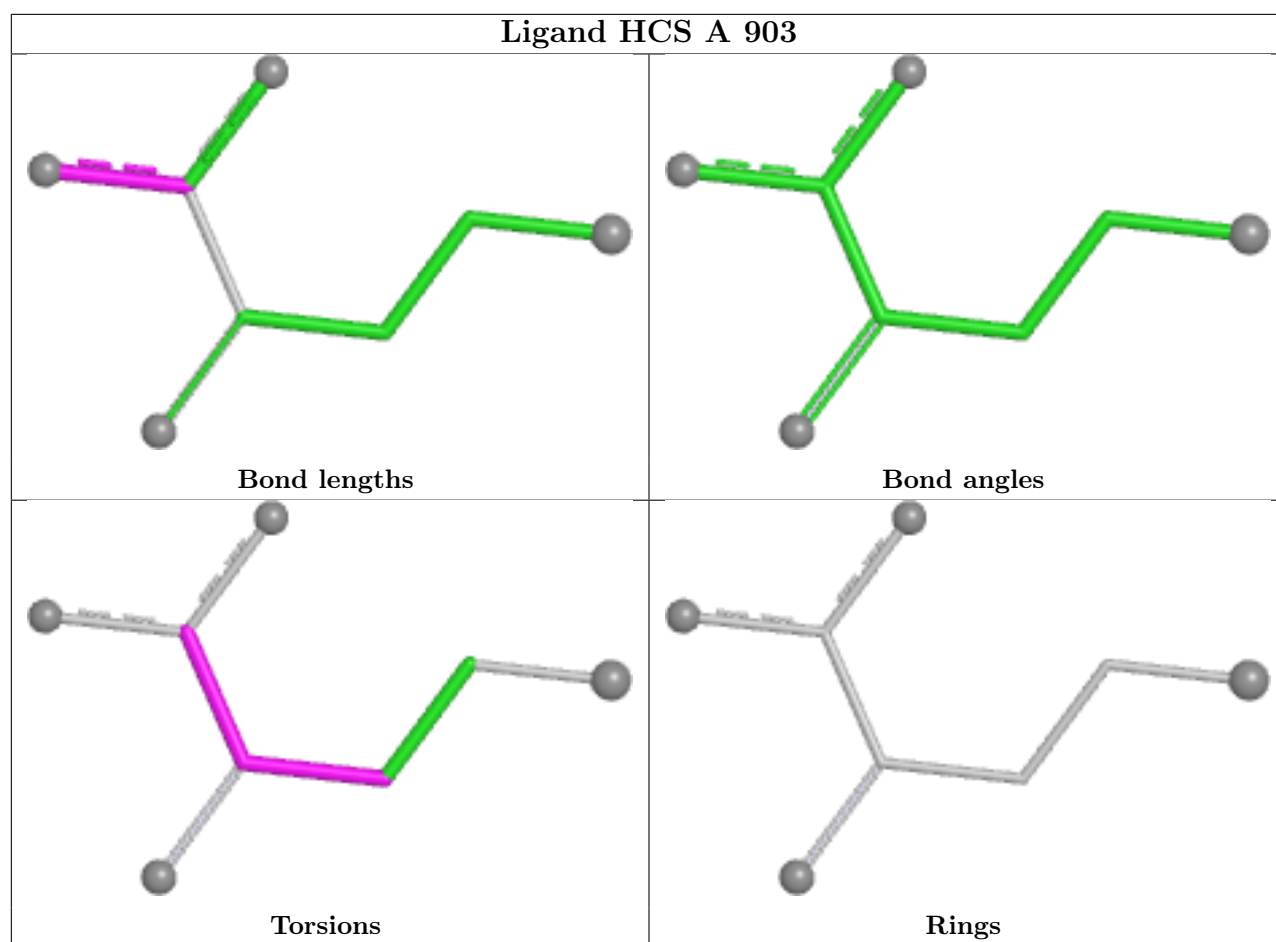
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	907	GOL	1	0
5	A	911	GOL	4	0
6	A	910	B12	13	0
8	A	914	TME	2	0

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

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	862/877 (98%)	0.43	37 (4%) 40 39	32, 67, 98, 145	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	ASN	4.4
1	A	747	GLY	4.1
1	A	2	VAL	4.1
1	A	524[A]	ARG	3.9
1	A	870	LEU	3.5
1	A	4	VAL	3.4
1	A	22	ASP	3.4
1	A	744	LYS	3.3
1	A	539	GLN	3.2
1	A	743	LYS	3.1
1	A	1	MET	3.1
1	A	540	GLY	3.0
1	A	874	ALA	2.9
1	A	368	LEU	2.8
1	A	62	LYS	2.8
1	A	508	ARG	2.7
1	A	634	GLY	2.7
1	A	867	MET	2.7
1	A	477	ARG	2.6
1	A	811	LYS	2.5
1	A	650	GLU	2.4
1	A	579	LYS	2.4
1	A	633	GLU	2.4
1	A	814	LEU	2.2
1	A	839	LEU	2.2
1	A	61	GLN	2.2
1	A	873	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	617	GLU	2.2
1	A	872	GLY	2.2
1	A	654	LYS	2.2
1	A	284	ALA	2.1
1	A	3	GLU	2.1
1	A	865	ARG	2.1
1	A	541	ASP	2.1
1	A	746	GLU	2.1
1	A	338	LYS	2.0
1	A	469	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

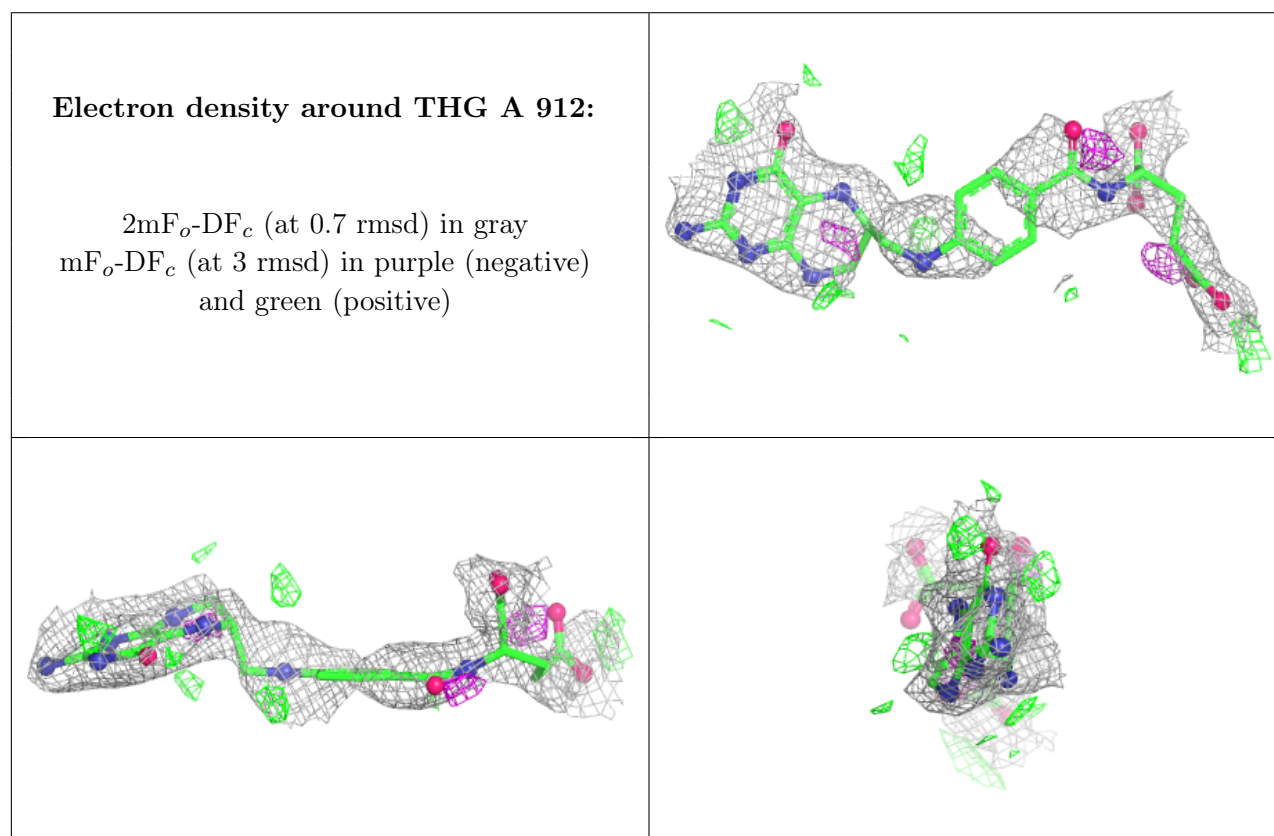
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	911	6/6	0.76	0.26	81,105,120,129	0
7	THG	A	912	32/32	0.80	0.20	61,90,115,126	32
8	TME	A	914	3/3	0.85	0.31	73,73,74,88	0
5	GOL	A	904	6/6	0.86	0.26	62,74,91,103	0
5	GOL	A	909	6/6	0.89	0.18	64,80,89,91	0
5	GOL	A	906	6/6	0.89	0.18	77,83,96,98	0
6	B12	A	910	91/91	0.90	0.16	43,65,83,94	0
4	HCS	A	903	8/8	0.92	0.14	73,80,96,98	0
5	GOL	A	907	6/6	0.94	0.13	61,79,87,93	0
5	GOL	A	905	6/6	0.94	0.11	58,67,75,100	0
5	GOL	A	908	6/6	0.95	0.11	65,76,101,102	0
3	K	A	902	1/1	0.97	0.12	67,67,67,67	0
2	ZN	A	901	1/1	0.98	0.10	80,80,80,80	0

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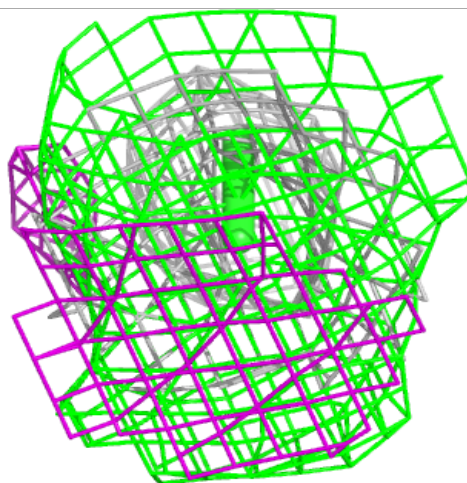
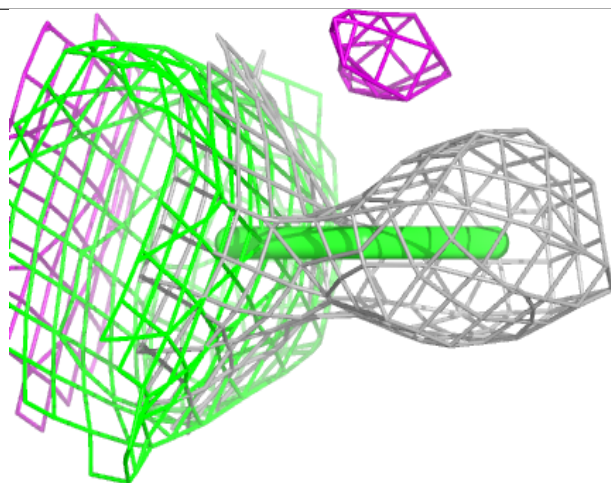
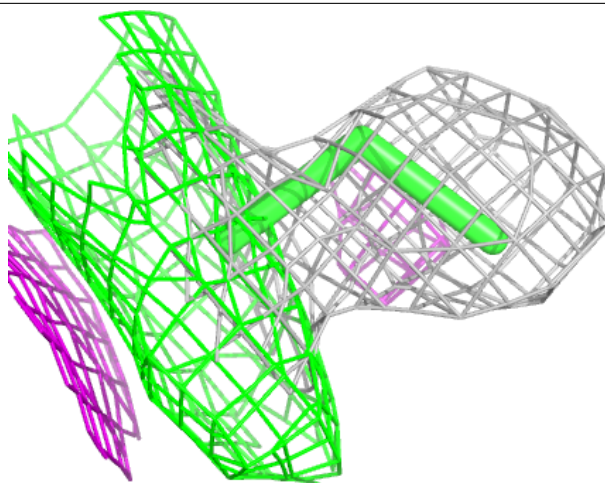
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	913	1/1	0.99	0.03	61,61,61,61	0

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.



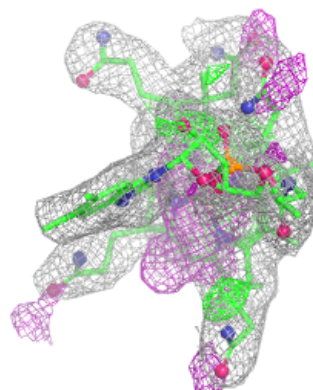
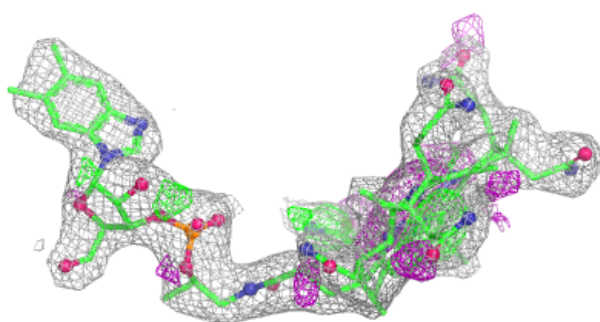
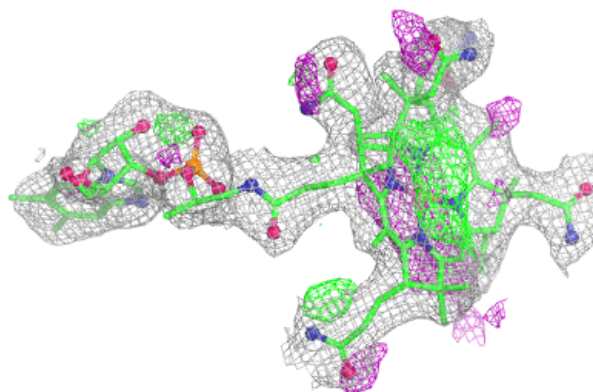
Electron density around TME A 914:

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

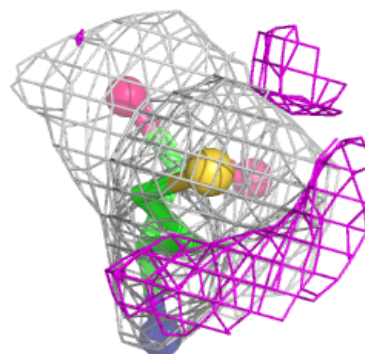
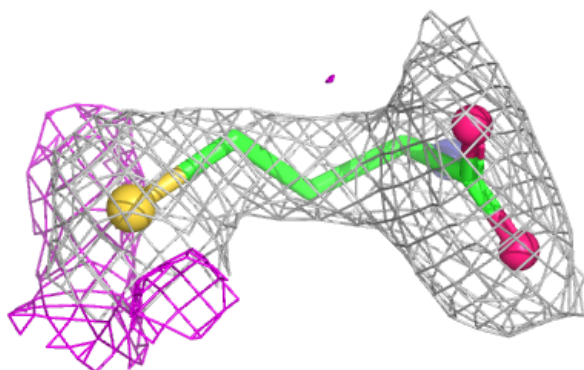
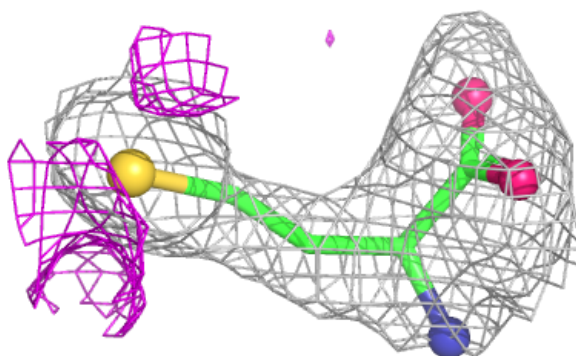


Electron density around B12 A 910:

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

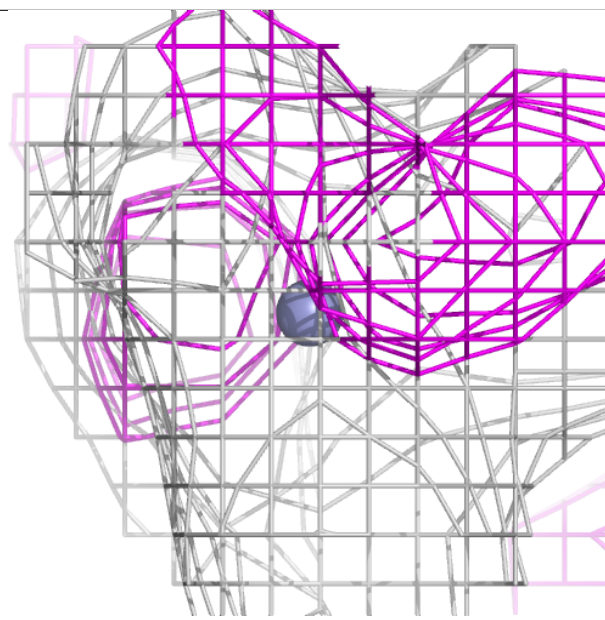
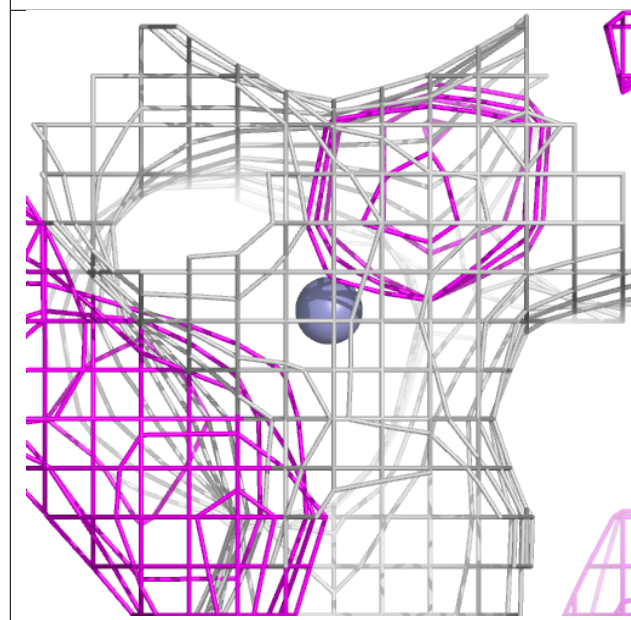
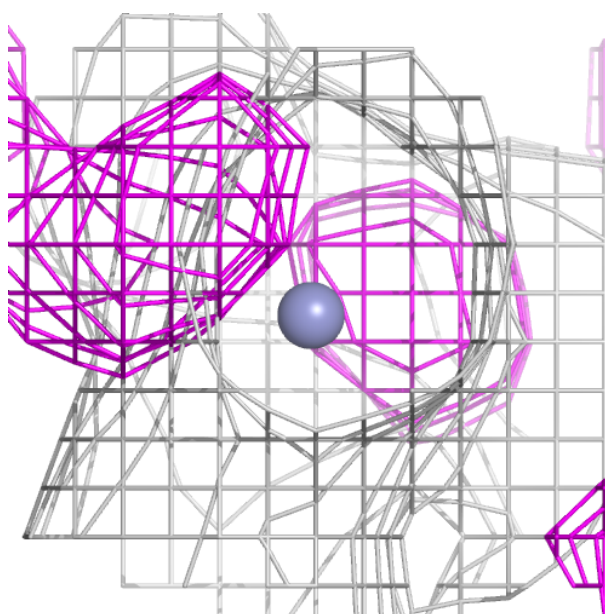
**Electron density around HCS A 903:**

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



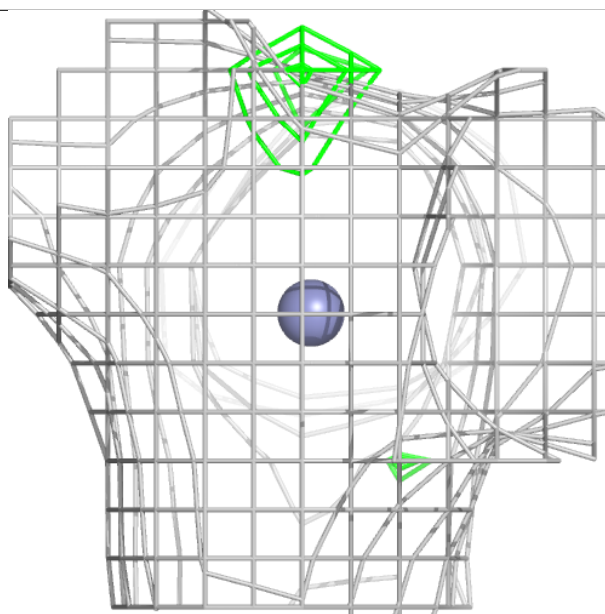
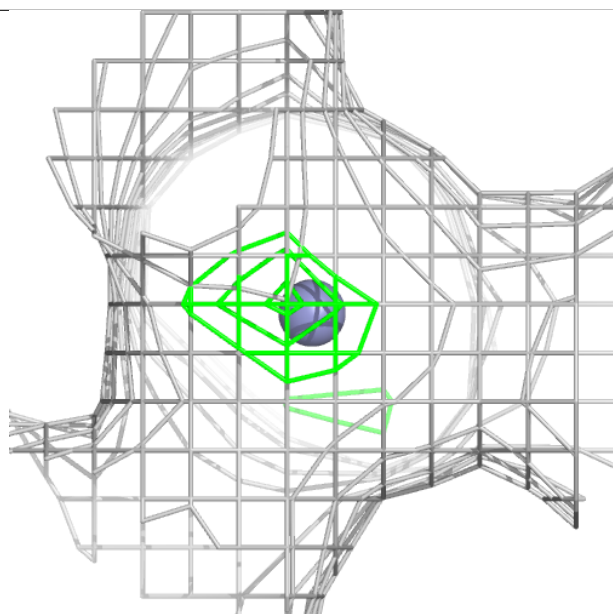
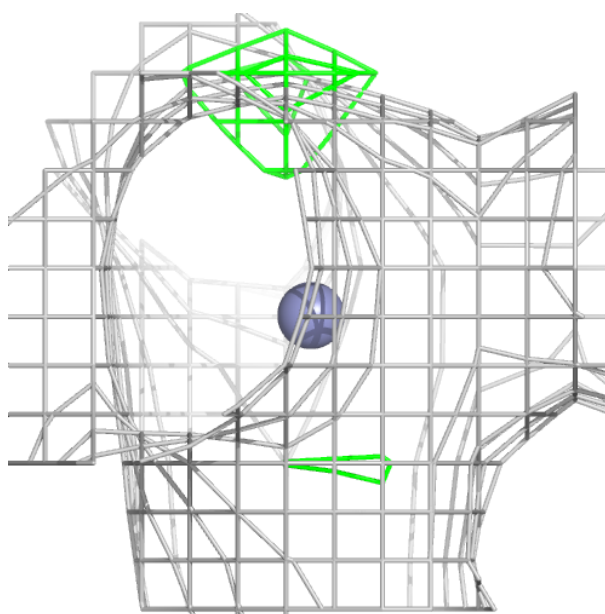
Electron density around ZN A 901:

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



Electron density around ZN A 913:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.