



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:43 PM UTC

PDB ID : 6TI3 / pdb_00006ti3
Title : Apo-SHMT from Streptococcus thermophilus Tyr55Ser variant in complex with D-Threonine
Authors : Petrillo, G.; Hernandez, K.; Bujons, J.; Clapes, P.; Uson, I.
Deposited on : 2019-11-21
Resolution : 1.96 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

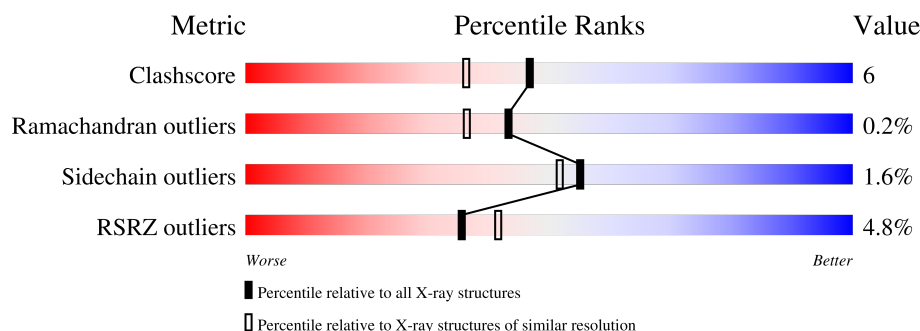
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	416	5% 82% 15% ..
1	B	416	4% 88% 10% ..
1	C	416	2% 82% 13% ..
1	D	416	7% 82% 15% ..

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
2	GOL	C	501	-	X	-	-
3	DTH	A	502	-	-	X	-
3	DTH	B	502	-	-	X	-
3	DTH	C	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13368 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 Serine hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	1	0
			3127	1978	538	602	9			
1	C	410	Total	C	N	O	S	0	1	0
			3119	1974	536	600	9			
1	B	410	Total	C	N	O	S	0	1	0
			3127	1978	538	602	9			
1	D	410	Total	C	N	O	S	0	1	0
			3119	1974	536	600	9			

There are 4 discrepancies between the modelled and reference sequences:

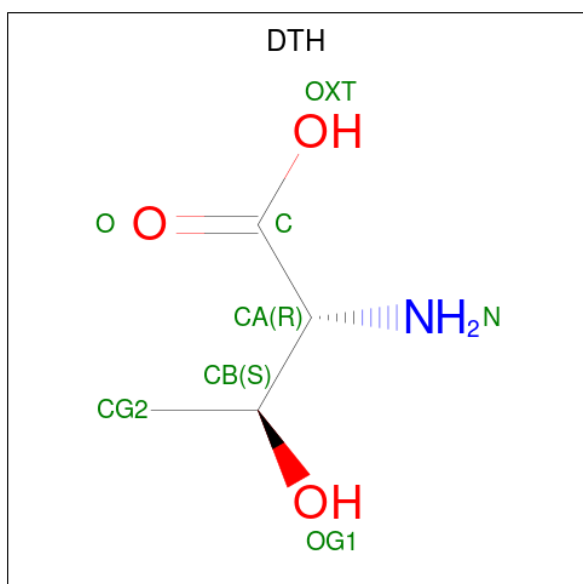
Chain	Residue	Modelled	Actual	Comment	Reference
A	55	SER	TYR	engineered mutation	UNP Q5MCK9
C	55	SER	TYR	engineered mutation	UNP Q5MCK9
B	55	SER	TYR	engineered mutation	UNP Q5MCK9
D	55	SER	TYR	engineered mutation	UNP Q5MCK9

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is D-THREONINE (CCD ID: DTH) (formula: $C_4H_9NO_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		

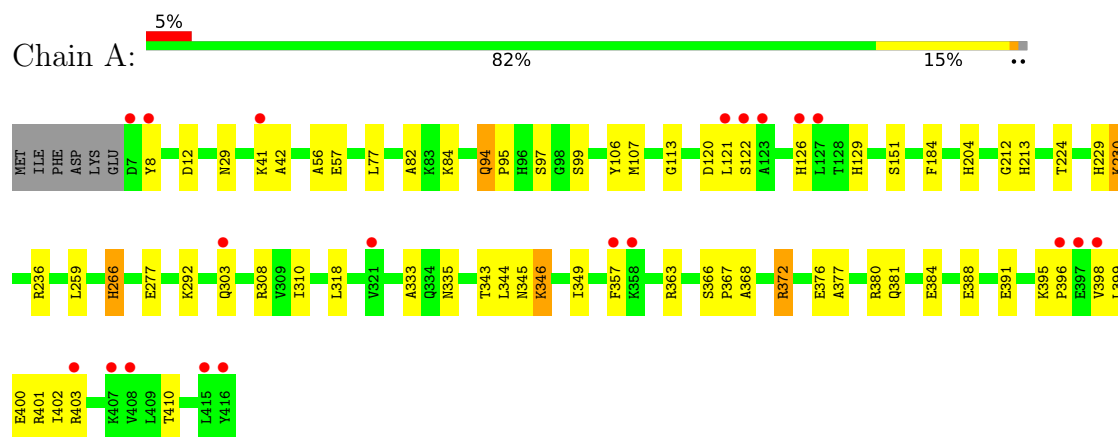
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	237	Total	O	0	0
			237	237		
5	C	232	Total	O	0	0
			232	232		
5	B	220	Total	O	0	0
			220	220		
5	D	136	Total	O	0	0
			136	136		

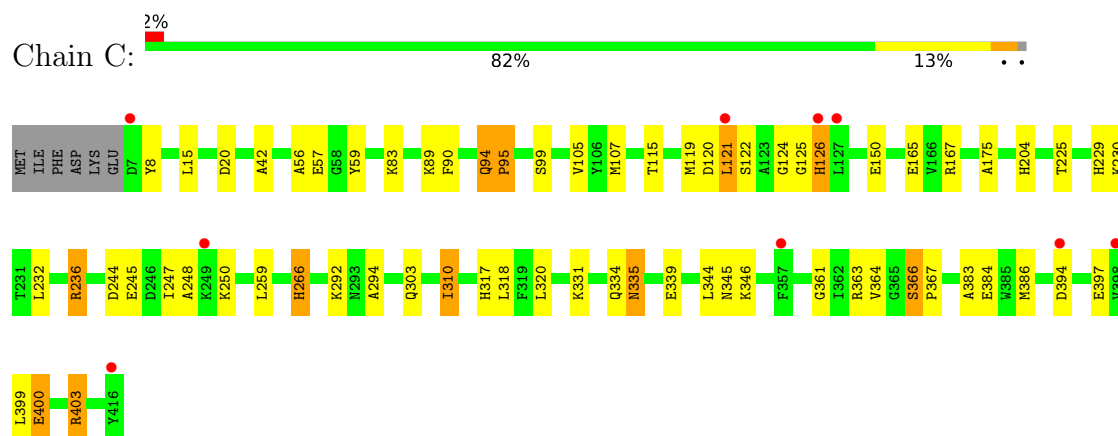
3 Residue-property plots [i](#)

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.

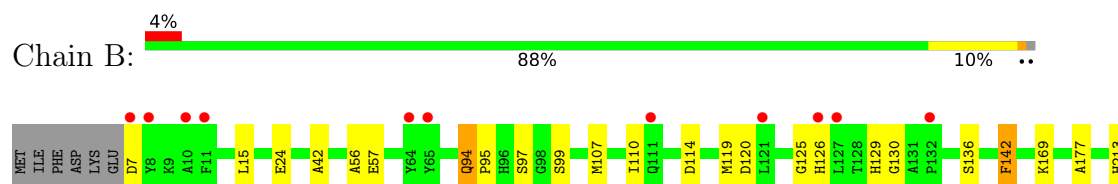
- Molecule 1: Serine hydroxymethyltransferase

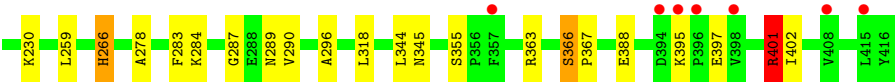


- Molecule 1: Serine hydroxymethyltransferase

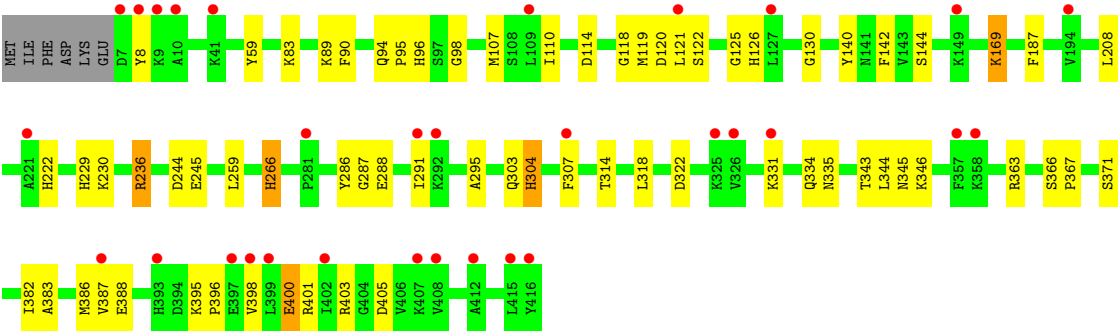
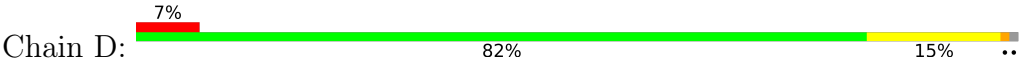


- Molecule 1: Serine hydroxymethyltransferase





● Molecule 1: Serine hydroxymethyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	200.39Å 113.69Å 133.15Å 90.00° 94.51° 90.00°	Depositor
Resolution (Å)	100.09 – 1.96 100.09 – 2.14	Depositor EDS
% Data completeness (in resolution range)	98.8 (100.09-1.96) 99.0 (100.09-2.14)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.181 , (Not available) 0.181 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13368	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DTH, GOL

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	1.40	28/3189 (0.9%)	1.31	9/4330 (0.2%)
1	B	1.26	14/3189 (0.4%)	1.22	10/4330 (0.2%)
1	C	1.36	14/3188 (0.4%)	1.28	14/4328 (0.3%)
1	D	1.13	7/3188 (0.2%)	1.20	5/4328 (0.1%)
All	All	1.29	63/12754 (0.5%)	1.26	38/17316 (0.2%)

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	4
1	B	0	1
1	C	0	3
1	D	0	1
All	All	0	9

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	292	LYS	N-CA	9.22	1.57	1.46
1	C	384	GLU	N-CA	8.56	1.56	1.46
1	C	364	VAL	N-CA	-7.76	1.37	1.46
1	A	292	LYS	N-CA	7.66	1.55	1.46
1	A	230	LYS	N-CA	7.21	1.55	1.46
1	C	361	GLY	N-CA	7.02	1.51	1.45
1	A	184	PHE	C-O	6.96	1.32	1.24
1	B	284	LYS	C-O	6.91	1.32	1.24
1	A	224	THR	C-O	6.90	1.32	1.24
1	D	288	GLU	N-CA	6.85	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110	ILE	N-CA	6.30	1.53	1.45
1	A	333	ALA	C-O	6.26	1.31	1.24
1	B	129	HIS	CE1-NE2	6.22	1.38	1.32
1	A	82	ALA	N-CA	6.22	1.53	1.46
1	D	59	TYR	N-CA	6.21	1.51	1.45
1	C	399	LEU	N-CA	6.13	1.53	1.46
1	C	294	ALA	C-O	6.04	1.31	1.24
1	B	213	HIS	CE1-NE2	5.99	1.38	1.32
1	B	114	ASP	N-CA	5.99	1.53	1.45
1	D	295	ALA	N-CA	5.98	1.53	1.46
1	B	142	PHE	C-O	-5.98	1.16	1.24
1	D	398	VAL	N-CA	5.98	1.53	1.46
1	B	296	ALA	N-CA	5.95	1.53	1.46
1	A	129	HIS	CE1-NE2	5.92	1.38	1.32
1	D	222	HIS	CE1-NE2	5.92	1.38	1.32
1	D	314	THR	C-O	-5.84	1.16	1.23
1	A	94	GLN	N-CA	5.83	1.54	1.46
1	C	232	LEU	C-O	-5.81	1.16	1.24
1	A	381	GLN	C-O	5.80	1.30	1.24
1	A	84	LYS	N-CA	-5.79	1.39	1.46
1	A	106	TYR	N-CA	5.78	1.53	1.46
1	A	372	ARG	N-CA	5.72	1.53	1.46
1	C	335	ASN	N-CA	5.70	1.53	1.46
1	A	277	GLU	N-CA	5.63	1.53	1.46
1	B	177	ALA	C-O	-5.63	1.16	1.24
1	C	250	LYS	N-CA	-5.61	1.39	1.46
1	A	113	GLY	N-CA	5.56	1.53	1.45
1	A	368	ALA	N-CA	5.55	1.53	1.46
1	A	213	HIS	CE1-NE2	5.49	1.38	1.32
1	C	394	ASP	CB-CG	-5.48	1.38	1.52
1	A	377	ALA	N-CA	5.43	1.52	1.46
1	D	187	PHE	N-CA	5.43	1.52	1.46
1	A	398	VAL	N-CA	5.42	1.53	1.46
1	A	402	ILE	N-CA	5.42	1.52	1.46
1	A	410	THR	N-CA	5.37	1.52	1.46
1	A	151	SER	N-CA	5.37	1.53	1.46
1	B	289	ASN	N-CA	5.36	1.52	1.46
1	A	77	LEU	N-CA	-5.35	1.40	1.46
1	B	401	ARG	C-O	5.33	1.30	1.24
1	C	310	ILE	C-O	-5.25	1.18	1.24
1	B	94	GLN	N-CA	5.24	1.53	1.46
1	A	212	GLY	C-O	-5.18	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	402	ILE	N-CA	5.17	1.52	1.46
1	C	303	GLN	N-CA	5.17	1.52	1.46
1	C	59	TYR	N-CA	5.15	1.50	1.45
1	A	229	HIS	CE1-NE2	5.14	1.37	1.32
1	A	376	GLU	C-O	5.14	1.30	1.24
1	B	287	GLY	N-CA	5.10	1.52	1.45
1	A	399	LEU	N-CA	5.04	1.52	1.46
1	B	290	VAL	N-CA	5.04	1.52	1.46
1	A	12	ASP	N-CA	5.04	1.52	1.46
1	C	339	GLU	N-CA	5.03	1.52	1.46
1	A	335	ASN	N-CA	5.03	1.52	1.46

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	SER	CA-C-N	-8.85	109.23	119.05
1	B	366	SER	C-N-CA	-8.85	109.23	119.05
1	A	349	ILE	CA-C-N	-7.37	112.17	119.76
1	A	349	ILE	C-N-CA	-7.37	112.17	119.76
1	C	394	ASP	N-CA-C	6.76	120.98	112.87
1	C	20	ASP	N-CA-C	-6.47	104.31	111.36
1	C	204	HIS	CA-CB-CG	-6.27	107.53	113.80
1	C	394	ASP	CB-CA-C	-6.19	96.66	110.21
1	D	395	LYS	CA-C-N	6.15	127.53	119.84
1	D	395	LYS	C-N-CA	6.15	127.53	119.84
1	B	120	ASP	CA-C-N	6.09	129.28	120.38
1	B	120	ASP	C-N-CA	6.09	129.28	120.38
1	A	344	LEU	CA-C-O	-5.91	115.10	121.36
1	A	395	LYS	CA-C-N	5.83	127.12	119.84
1	A	395	LYS	C-N-CA	5.83	127.12	119.84
1	C	397	GLU	CB-CG-CD	5.59	122.11	112.60
1	B	94	GLN	CA-C-N	-5.54	114.25	119.90
1	B	94	GLN	C-N-CA	-5.54	114.25	119.90
1	C	126	HIS	CA-CB-CG	5.52	119.32	113.80
1	D	304	HIS	CB-CA-C	5.52	118.36	109.41
1	B	126	HIS	CA-CB-CG	5.49	119.29	113.80
1	C	115	THR	CA-CB-OG1	-5.49	101.37	109.60
1	B	136	SER	CA-C-N	5.48	126.99	120.14
1	B	136	SER	C-N-CA	5.48	126.99	120.14
1	C	94	GLN	CA-C-N	-5.46	114.33	119.90
1	C	94	GLN	C-N-CA	-5.46	114.33	119.90
1	D	304	HIS	CA-C-N	5.41	125.02	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	304	HIS	C-N-CA	5.41	125.02	119.56
1	C	150	GLU	CB-CG-CD	5.29	121.59	112.60
1	C	95	PRO	CB-CA-C	-5.28	104.85	111.56
1	A	94	GLN	CA-C-N	-5.26	114.34	119.76
1	A	94	GLN	C-N-CA	-5.26	114.34	119.76
1	C	366	SER	CA-C-N	-5.25	113.22	119.05
1	C	366	SER	C-N-CA	-5.25	113.22	119.05
1	A	204	HIS	CA-CB-CG	-5.24	108.56	113.80
1	B	344	LEU	CA-C-O	-5.20	115.19	121.32
1	A	126	HIS	CA-CB-CG	5.11	118.91	113.80
1	C	165	GLU	CB-CA-C	-5.07	102.89	110.90

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	ARG	Sidechain
1	A	308	ARG	Sidechain
1	A	372	ARG	Sidechain
1	A	403	ARG	Sidechain
1	B	401	ARG	Sidechain
1	C	167	ARG	Sidechain
1	C	236	ARG	Sidechain
1	C	403	ARG	Sidechain
1	D	236	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	3127	0	3106	29	0
1	B	3127	0	3106	24	0
1	C	3119	0	3093	45	0
1	D	3119	0	3093	46	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	8	6	0
3	B	8	0	8	6	0
3	C	8	0	8	6	0
3	D	8	0	8	2	0
4	D	1	0	0	0	0
5	A	237	0	0	5	0
5	B	220	0	0	4	0
5	C	232	0	0	1	0
5	D	136	0	0	2	1
All	All	13368	0	12454	143	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 6.

All (143) 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:303:GLN:HG3	5:A:744:HOH:O	1.73	0.89
1:D:334:GLN:HE21	1:D:346:LYS:H	1.29	0.81
1:C:99:SER:OG	3:C:502:DTH:CG2	2.36	0.73
1:C:334:GLN:HE21	1:C:346:LYS:H	1.37	0.73
1:A:303:GLN:CG	5:A:744:HOH:O	2.32	0.71
1:C:121:LEU:HD22	1:C:121:LEU:H	1.54	0.70
1:D:400:GLU:OE2	1:D:403:ARG:NH2	2.24	0.70
1:B:99:SER:OG	3:B:502:DTH:CG2	2.40	0.69
1:C:266:HIS:H	1:C:266:HIS:CD2	2.10	0.69
1:D:266:HIS:CD2	1:D:266:HIS:H	2.14	0.66
1:D:383:ALA:HA	1:D:386:MET:HE3	1.79	0.65
1:C:99:SER:OG	3:C:502:DTH:HG22	1.97	0.64
1:B:99:SER:OG	3:B:502:DTH:HG22	1.99	0.61
1:A:99:SER:H	3:A:502:DTH:HG23	1.66	0.60
1:C:107:MET:HE1	1:C:259:LEU:HD21	1.83	0.60
1:A:97:SER:HB2	3:A:502:DTH:HG21	1.84	0.60
1:A:99:SER:H	3:A:502:DTH:CG2	2.16	0.59
1:B:107:MET:HE1	1:B:259:LEU:HG	1.85	0.59
1:A:318:LEU:C	1:A:318:LEU:HD12	2.28	0.57
1:D:120:ASP:OD2	1:D:122:SER:HB2	2.04	0.57
1:C:99:SER:N	3:C:502:DTH:HG23	2.21	0.56
1:C:99:SER:H	3:C:502:DTH:CG2	2.19	0.56
1:D:401:ARG:HD2	1:D:405:ASP:OD2	2.06	0.56
1:C:121:LEU:HD22	1:C:121:LEU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:GLN:NE2	1:D:346:LYS:H	2.00	0.55
1:B:345:ASN:HD21	1:B:363:ARG:HE	1.54	0.55
1:C:383:ALA:HA	1:C:386:MET:HE3	1.89	0.55
1:D:331:LYS:HE3	1:D:335:ASN:HD21	1.71	0.55
1:B:97:SER:HB2	3:B:502:DTH:HG21	1.88	0.55
1:C:121:LEU:H	1:C:121:LEU:CD2	2.18	0.54
1:D:98:GLY:H	3:D:502:DTH:HG21	1.72	0.54
1:D:366:SER:N	1:D:367:PRO:CD	2.71	0.54
1:C:107:MET:HE1	1:C:259:LEU:CD2	2.38	0.54
1:B:397:GLU:OE1	1:B:397:GLU:N	2.25	0.54
1:C:99:SER:H	3:C:502:DTH:HG23	1.73	0.53
1:B:266:HIS:H	1:B:266:HIS:CD2	2.24	0.53
1:A:99:SER:N	3:A:502:DTH:HG23	2.23	0.53
1:A:107:MET:HE1	1:A:259:LEU:HG	1.91	0.53
1:A:266:HIS:H	1:A:266:HIS:CD2	2.26	0.53
1:B:99:SER:H	3:B:502:DTH:CG2	2.22	0.53
1:C:90:PHE:CZ	1:C:245:GLU:HG3	2.44	0.52
1:A:29:ASN:HD21	1:A:343:THR:HG23	1.74	0.52
1:A:345:ASN:ND2	5:A:603:HOH:O	2.42	0.52
1:D:344:LEU:C	1:D:344:LEU:HD12	2.34	0.52
1:A:345:ASN:HD21	1:A:363:ARG:HE	1.58	0.52
1:D:118:GLY:O	1:D:144:SER:HA	2.10	0.52
1:C:345:ASN:HD21	1:C:363:ARG:HH21	1.58	0.52
1:D:322:ASP:C	1:D:322:ASP:OD1	2.52	0.52
1:C:126:HIS:HB3	5:C:801:HOH:O	2.10	0.51
1:D:244:ASP:OD1	1:D:244:ASP:C	2.54	0.51
1:D:382:ILE:HG22	1:D:386:MET:HE2	1.92	0.50
1:A:99:SER:OG	3:A:502:DTH:CG2	2.60	0.50
1:B:42:ALA:HB2	1:D:8:TYR:HB2	1.93	0.50
1:C:318:LEU:C	1:C:318:LEU:HD12	2.36	0.50
1:D:287:GLY:O	1:D:291:ILE:HG12	2.12	0.50
1:D:208:LEU:HD13	1:D:291:ILE:HD11	1.92	0.50
1:D:388:GLU:OE2	1:D:401:ARG:NH1	2.45	0.50
1:D:107:MET:HE1	1:D:259:LEU:HD21	1.93	0.50
1:A:346:LYS:HE3	1:A:357:PHE:O	2.11	0.49
1:A:380:ARG:O	1:A:384:GLU:HG2	2.12	0.49
1:D:401:ARG:NH2	1:D:405:ASP:OD2	2.34	0.49
1:B:56:ALA:O	1:B:57:GLU:C	2.53	0.48
1:D:345:ASN:HD21	1:D:363:ARG:HH21	1.61	0.48
1:C:400:GLU:OE2	1:C:403:ARG:NH1	2.46	0.48
1:D:83:LYS:HE3	1:D:89:LYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:PHE:CZ	1:D:245:GLU:HG3	2.49	0.48
1:C:266:HIS:H	1:C:266:HIS:HD2	1.61	0.48
1:B:15:LEU:C	1:B:15:LEU:HD13	2.39	0.48
1:D:94:GLN:N	1:D:95:PRO:CD	2.77	0.47
1:D:121:LEU:HD22	1:D:121:LEU:N	2.30	0.47
1:C:107:MET:HE1	1:C:259:LEU:CG	2.45	0.47
1:C:266:HIS:CD2	1:C:266:HIS:N	2.82	0.47
1:C:99:SER:OG	3:C:502:DTH:HG23	2.15	0.46
1:D:107:MET:HE1	1:D:259:LEU:CD2	2.45	0.46
1:C:119:MET:O	1:C:125:GLY:HA3	2.15	0.46
1:C:334:GLN:NE2	1:C:346:LYS:H	2.07	0.46
2:C:501:GOL:H11	5:B:719:HOH:O	2.15	0.46
1:A:42:ALA:HB2	1:C:8:TYR:HB2	1.96	0.46
1:D:345:ASN:ND2	1:D:363:ARG:HH21	2.13	0.46
1:A:388:GLU:OE2	1:A:401:ARG:NH1	2.45	0.46
1:C:56:ALA:O	1:C:57:GLU:C	2.55	0.46
1:B:107:MET:HE1	1:B:259:LEU:CG	2.45	0.46
1:B:130:GLY:HA3	1:B:142:PHE:CG	2.51	0.46
1:D:126:HIS:HB3	5:D:711:HOH:O	2.16	0.45
1:C:107:MET:HE1	1:C:259:LEU:HG	1.98	0.45
1:A:107:MET:HE1	1:A:259:LEU:CG	2.46	0.45
1:C:400:GLU:HG2	1:C:403:ARG:HH12	1.82	0.45
1:D:318:LEU:HD12	1:D:318:LEU:C	2.41	0.45
1:C:345:ASN:ND2	1:C:363:ARG:HH21	2.15	0.45
1:C:83:LYS:HE3	1:C:89:LYS:O	2.16	0.45
1:B:318:LEU:C	1:B:318:LEU:HD12	2.42	0.44
1:C:244:ASP:OD1	1:C:244:ASP:C	2.60	0.44
1:B:119:MET:O	1:B:125:GLY:HA3	2.17	0.44
1:D:266:HIS:H	1:D:266:HIS:HD2	1.62	0.44
1:A:391:GLU:CG	5:A:601:HOH:O	2.65	0.44
1:C:247:ILE:O	1:C:248:ALA:C	2.59	0.44
1:A:107:MET:HE1	1:A:259:LEU:CD2	2.48	0.44
1:A:56:ALA:O	1:A:57:GLU:C	2.61	0.44
1:C:331:LYS:HE3	1:C:335:ASN:HD21	1.83	0.44
1:B:366:SER:N	1:B:367:PRO:CD	2.81	0.43
1:B:107:MET:HE1	1:B:259:LEU:CD2	2.49	0.43
1:B:345:ASN:ND2	5:B:612:HOH:O	2.51	0.43
1:D:119:MET:O	1:D:125:GLY:HA3	2.19	0.43
1:A:107:MET:HE1	1:A:259:LEU:HD21	1.99	0.43
1:D:388:GLU:CD	1:D:401:ARG:NH1	2.77	0.43
1:A:388:GLU:CD	1:A:401:ARG:HH12	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:GLN:N	1:C:95:PRO:CD	2.82	0.43
1:B:7:ASP:N	5:B:611:HOH:O	2.50	0.43
1:D:96:HIS:HD2	5:D:651:HOH:O	2.01	0.43
1:A:94:GLN:O	1:A:95:PRO:C	2.61	0.42
1:C:120:ASP:OD2	1:C:122:SER:HB2	2.19	0.42
1:C:317:HIS:NE2	1:C:318:LEU:HD23	2.34	0.42
1:D:229:HIS:ND1	1:D:236:ARG:HA	2.34	0.42
1:A:391:GLU:HG3	5:A:601:HOH:O	2.20	0.42
1:C:229:HIS:ND1	1:C:236:ARG:HA	2.35	0.42
1:D:110:ILE:HD12	1:D:140:TYR:CD1	2.54	0.42
1:D:307:PHE:CE2	1:D:387:VAL:HG22	2.55	0.42
1:D:304:HIS:CD2	1:D:387:VAL:HG11	2.54	0.42
1:C:15:LEU:C	1:C:15:LEU:HD13	2.45	0.42
1:D:114:ASP:CG	1:D:169:LYS:HE2	2.45	0.42
1:A:366:SER:N	1:A:367:PRO:CD	2.83	0.42
1:B:99:SER:N	3:B:502:DTH:HG23	2.35	0.41
1:D:130:GLY:HA3	1:D:142:PHE:CG	2.55	0.41
1:D:366:SER:H	1:D:367:PRO:HD3	1.86	0.41
1:B:388:GLU:OE2	1:B:401:ARG:NH1	2.53	0.41
1:A:8:TYR:HB2	1:C:42:ALA:HB2	2.03	0.41
1:A:120:ASP:OD2	1:A:122:SER:HB2	2.20	0.41
1:C:105:VAL:HG21	1:C:225:THR:CG2	2.50	0.41
1:C:124:GLY:O	1:C:175:ALA:HA	2.20	0.41
2:C:501:GOL:C1	5:B:719:HOH:O	2.69	0.41
1:C:310:ILE:HB	1:C:320:LEU:HB2	2.03	0.41
1:B:94:GLN:O	1:B:95:PRO:C	2.62	0.41
1:B:99:SER:H	3:B:502:DTH:HG23	1.84	0.41
1:D:229:HIS:CE1	3:D:502:DTH:HG22	2.56	0.41
1:A:99:SER:OG	3:A:502:DTH:HG22	2.20	0.41
1:C:107:MET:HE3	1:C:107:MET:HB2	1.81	0.41
1:D:388:GLU:CD	1:D:401:ARG:HH12	2.27	0.41
1:B:278:ALA:HA	1:B:283:PHE:CG	2.56	0.41
1:D:388:GLU:OE1	1:D:401:ARG:NH1	2.50	0.41
1:C:344:LEU:C	1:C:344:LEU:HD12	2.47	0.40
1:D:286:TYR:HE1	1:D:371:SER:HG	1.67	0.40
1:C:366:SER:N	1:C:367:PRO:CD	2.84	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)
5:D:664:HOH:O	5:D:705:HOH:O[2_656]	2.01	0.19

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	409/416 (98%)	394 (96%)	14 (3%)	1 (0%)	43	36
1	B	409/416 (98%)	401 (98%)	7 (2%)	1 (0%)	43	36
1	C	409/416 (98%)	399 (98%)	9 (2%)	1 (0%)	43	36
1	D	409/416 (98%)	394 (96%)	14 (3%)	1 (0%)	43	36
All	All	1636/1664 (98%)	1588 (97%)	44 (3%)	4 (0%)	43	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	LYS
1	C	230	LYS
1	B	230	LYS
1	D	230	LYS

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	328/333 (98%)	321 (98%)	7 (2%)	47	41
1	B	328/333 (98%)	322 (98%)	6 (2%)	51	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	328/333 (98%)	325 (99%)	3 (1%)	70	70
1	D	328/333 (98%)	323 (98%)	5 (2%)	57	54
All	All	1312/1332 (98%)	1291 (98%)	21 (2%)	55	52

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	121	LEU
1	A	266	HIS
1	A	310	ILE
1	A	346	LYS
1	A	396	PRO
1	A	400	GLU
1	C	121	LEU
1	C	266	HIS
1	C	400	GLU
1	B	24	GLU
1	B	169	LYS
1	B	266	HIS
1	B	355	SER
1	B	395	LYS
1	B	401	ARG
1	D	169	LYS
1	D	266	HIS
1	D	303	GLN
1	D	396	PRO
1	D	400	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	29	ASN
1	A	96	HIS
1	A	141	ASN
1	A	204	HIS
1	A	266	HIS
1	A	341	ASN
1	A	345	ASN

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Mol	Chain	Res	Type
1	A	347	ASN
1	A	381	GLN
1	C	17	ASN
1	C	96	HIS
1	C	141	ASN
1	C	204	HIS
1	C	266	HIS
1	C	334	GLN
1	C	335	ASN
1	C	341	ASN
1	C	345	ASN
1	C	347	ASN
1	C	381	GLN
1	B	17	ASN
1	B	266	HIS
1	B	303	GLN
1	B	341	ASN
1	B	345	ASN
1	B	347	ASN
1	B	353	GLN
1	B	381	GLN
1	D	17	ASN
1	D	96	HIS
1	D	111	GLN
1	D	141	ASN
1	D	266	HIS
1	D	334	GLN
1	D	335	ASN
1	D	341	ASN
1	D	345	ASN
1	D	381	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	C	501	-	5,5,5	1.54	1 (20%)	5,5,5	2.42	3 (60%)
3	DTH	A	502	-	7,7,7	1.27	1 (14%)	8,9,9	2.30	3 (37%)
3	DTH	C	502	-	7,7,7	0.85	0	8,9,9	2.33	5 (62%)
2	GOL	B	501	-	5,5,5	0.98	0	5,5,5	0.66	0
3	DTH	D	502	-	7,7,7	0.92	0	8,9,9	1.70	2 (25%)
2	GOL	A	501	-	5,5,5	0.48	0	5,5,5	0.58	0
3	DTH	B	502	-	7,7,7	1.45	1 (14%)	8,9,9	2.30	3 (37%)

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	GOL	C	501	-	-	2/4/4/4	-
3	DTH	A	502	-	-	2/8/8/8	-
3	DTH	C	502	-	-	2/8/8/8	-
2	GOL	B	501	-	-	0/4/4/4	-
3	DTH	D	502	-	-	4/8/8/8	-
2	GOL	A	501	-	-	0/4/4/4	-
3	DTH	B	502	-	-	0/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	DTH	OXT-C	-3.55	1.19	1.30
2	C	501	GOL	O2-C2	2.94	1.51	1.43
3	A	502	DTH	OXT-C	-2.91	1.21	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	GOL	C3-C2-C1	-4.43	95.55	111.80
3	A	502	DTH	OXT-C-O	-4.23	114.49	124.08
3	B	502	DTH	OXT-C-O	-4.00	114.99	124.08
3	C	502	DTH	OXT-C-CA	3.70	126.90	114.15
3	B	502	DTH	C-CA-N	3.50	116.85	109.49
3	C	502	DTH	OG1-CB-CG2	3.47	120.05	109.68
3	A	502	DTH	OG1-CB-CA	3.36	116.17	109.00
3	D	502	DTH	OXT-C-CA	3.36	125.72	114.15
3	D	502	DTH	OXT-C-O	-2.77	117.79	124.08
3	A	502	DTH	O-C-CA	2.73	130.97	121.72
3	B	502	DTH	OG1-CB-CA	2.59	114.51	109.00
3	C	502	DTH	OG1-CB-CA	2.38	114.07	109.00
3	C	502	DTH	OXT-C-O	-2.33	118.79	124.08
3	C	502	DTH	O-C-CA	-2.33	113.83	121.72
2	C	501	GOL	O2-C2-C3	2.13	117.99	109.18
2	C	501	GOL	O3-C3-C2	2.12	119.92	110.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

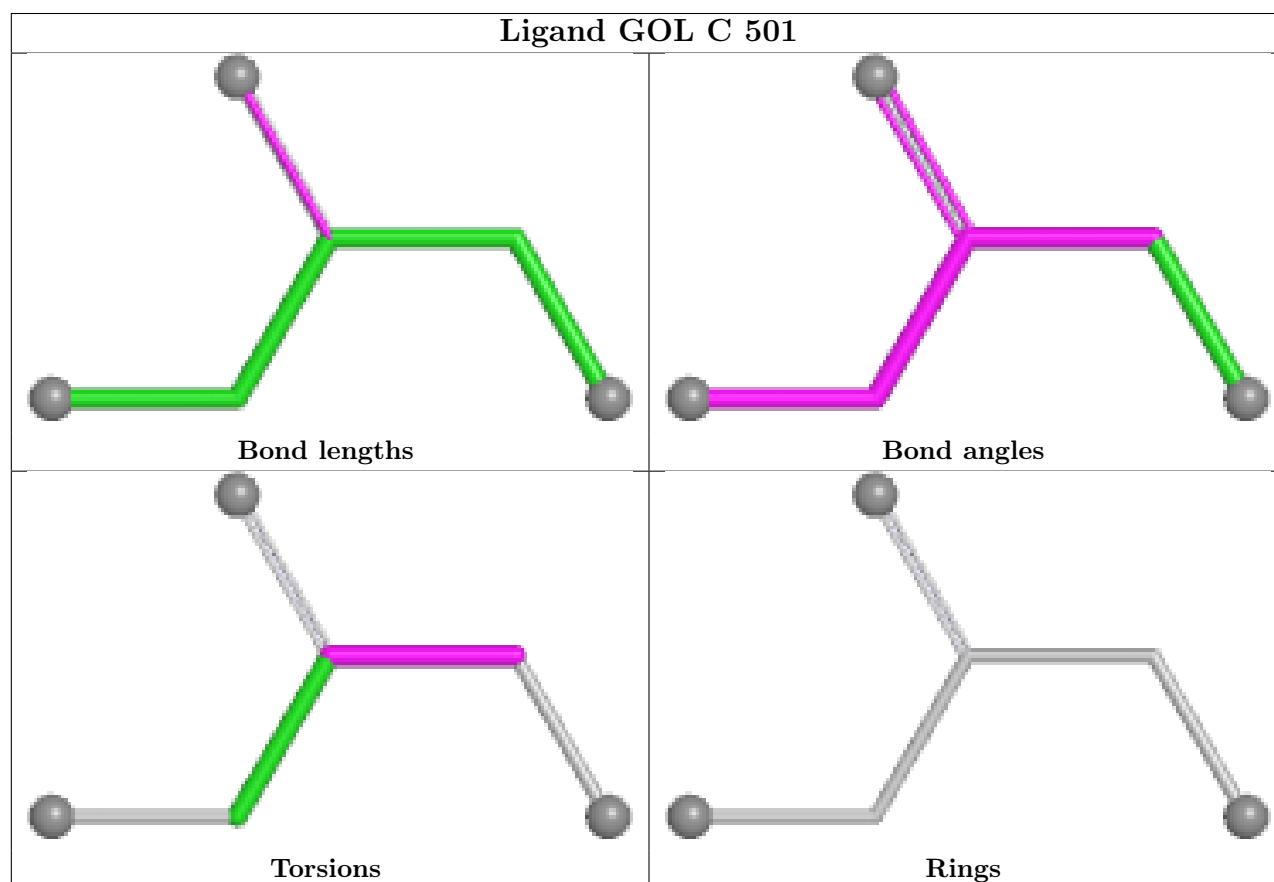
Mol	Chain	Res	Type	Atoms
3	A	502	DTH	C-CA-CB-CG2
3	C	502	DTH	C-CA-CB-CG2
3	D	502	DTH	N-CA-CB-CG2
3	D	502	DTH	N-CA-CB-OG1
3	D	502	DTH	C-CA-CB-CG2
3	D	502	DTH	C-CA-CB-OG1
2	C	501	GOL	O1-C1-C2-C3
2	C	501	GOL	O1-C1-C2-O2
3	A	502	DTH	N-CA-CB-CG2
3	C	502	DTH	N-CA-CB-CG2

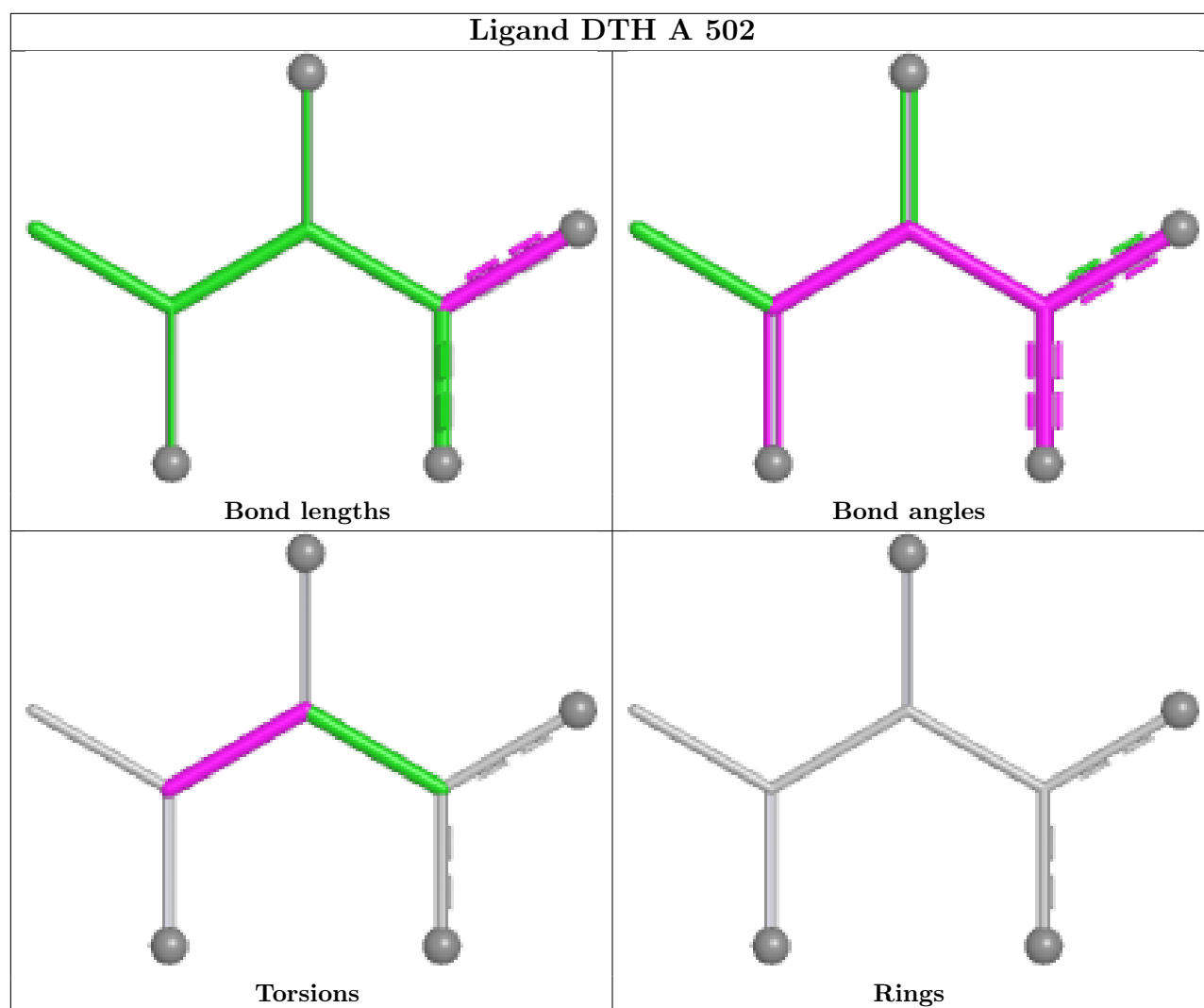
There are no ring outliers.

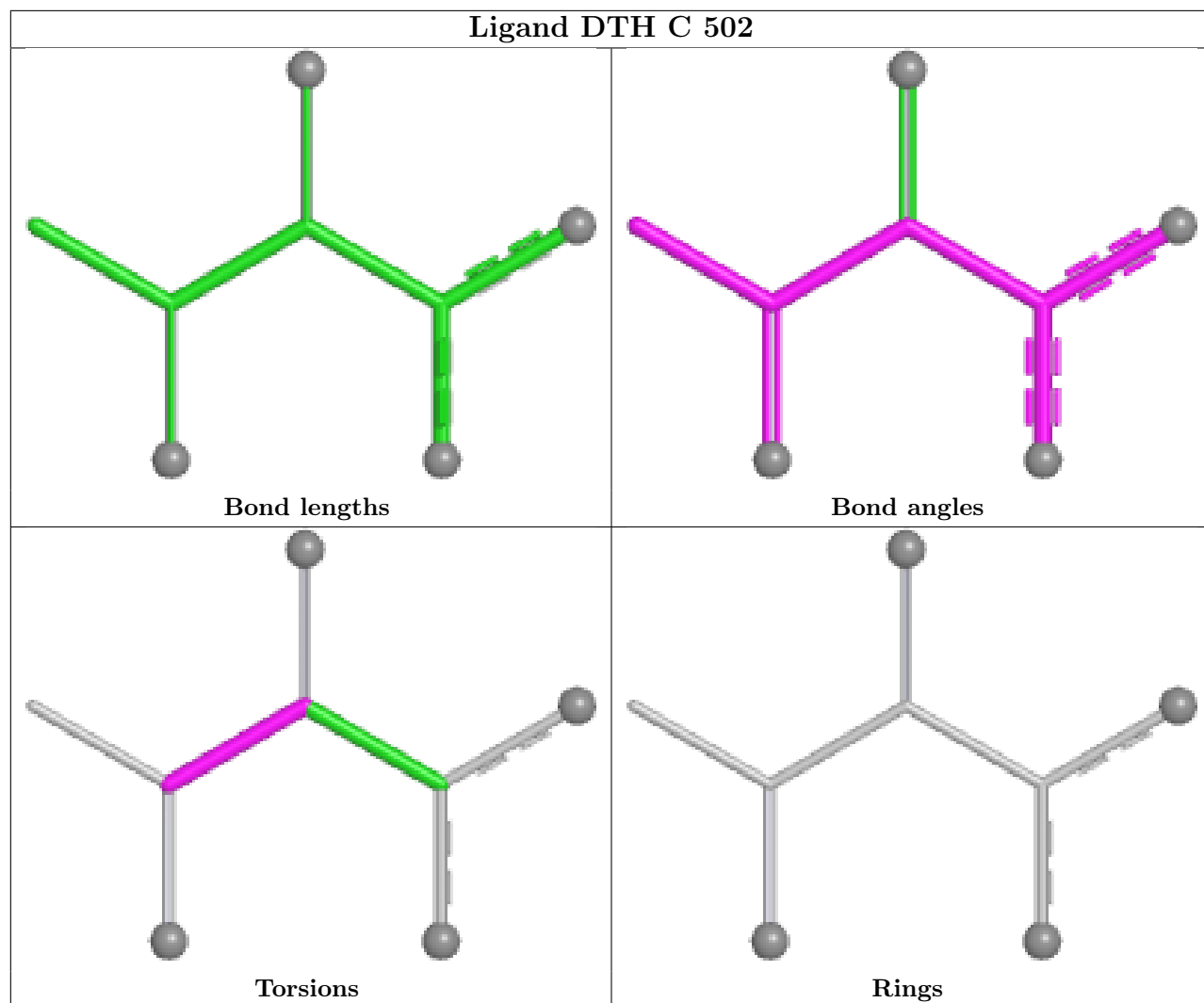
5 monomers are involved in 22 short contacts:

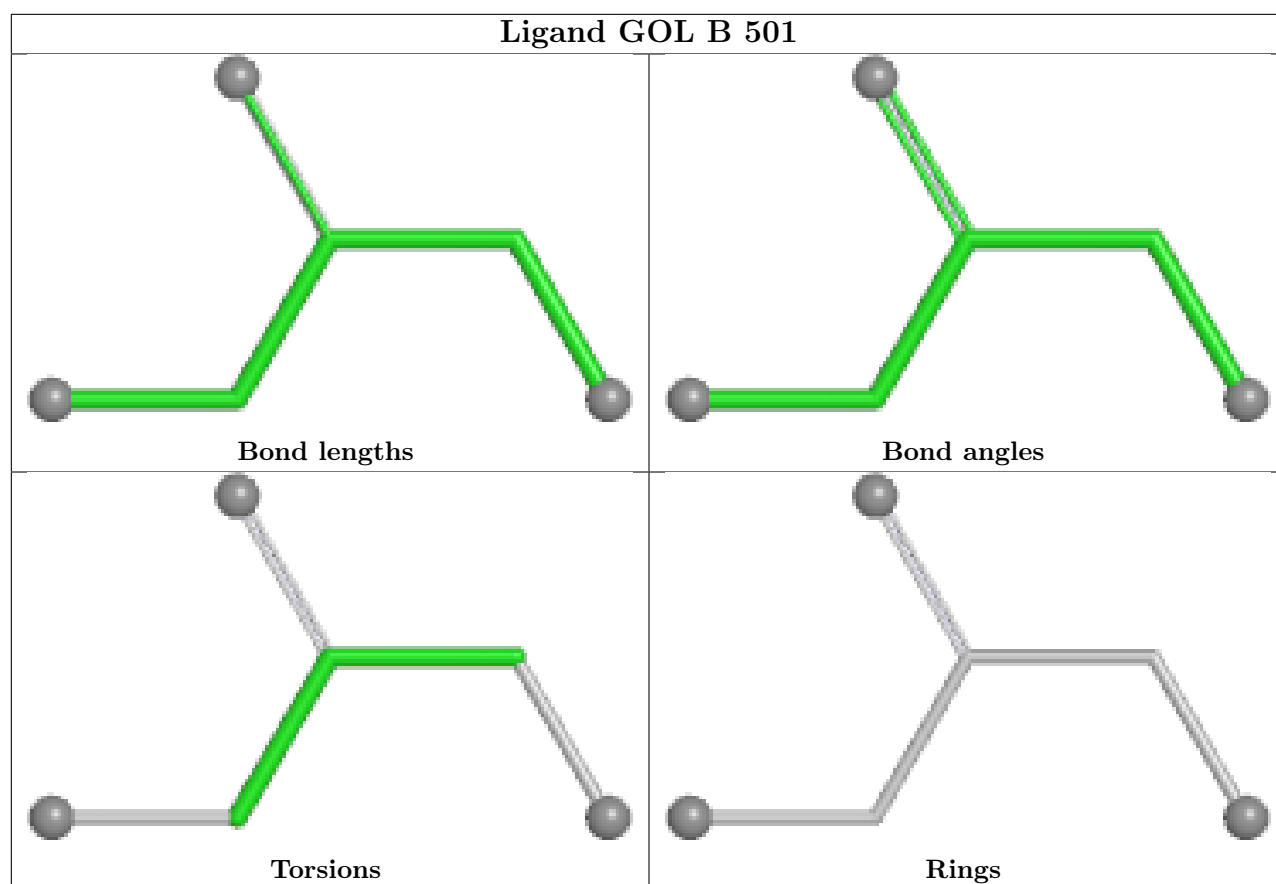
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	GOL	2	0
3	A	502	DTH	6	0
3	C	502	DTH	6	0
3	D	502	DTH	2	0
3	B	502	DTH	6	0

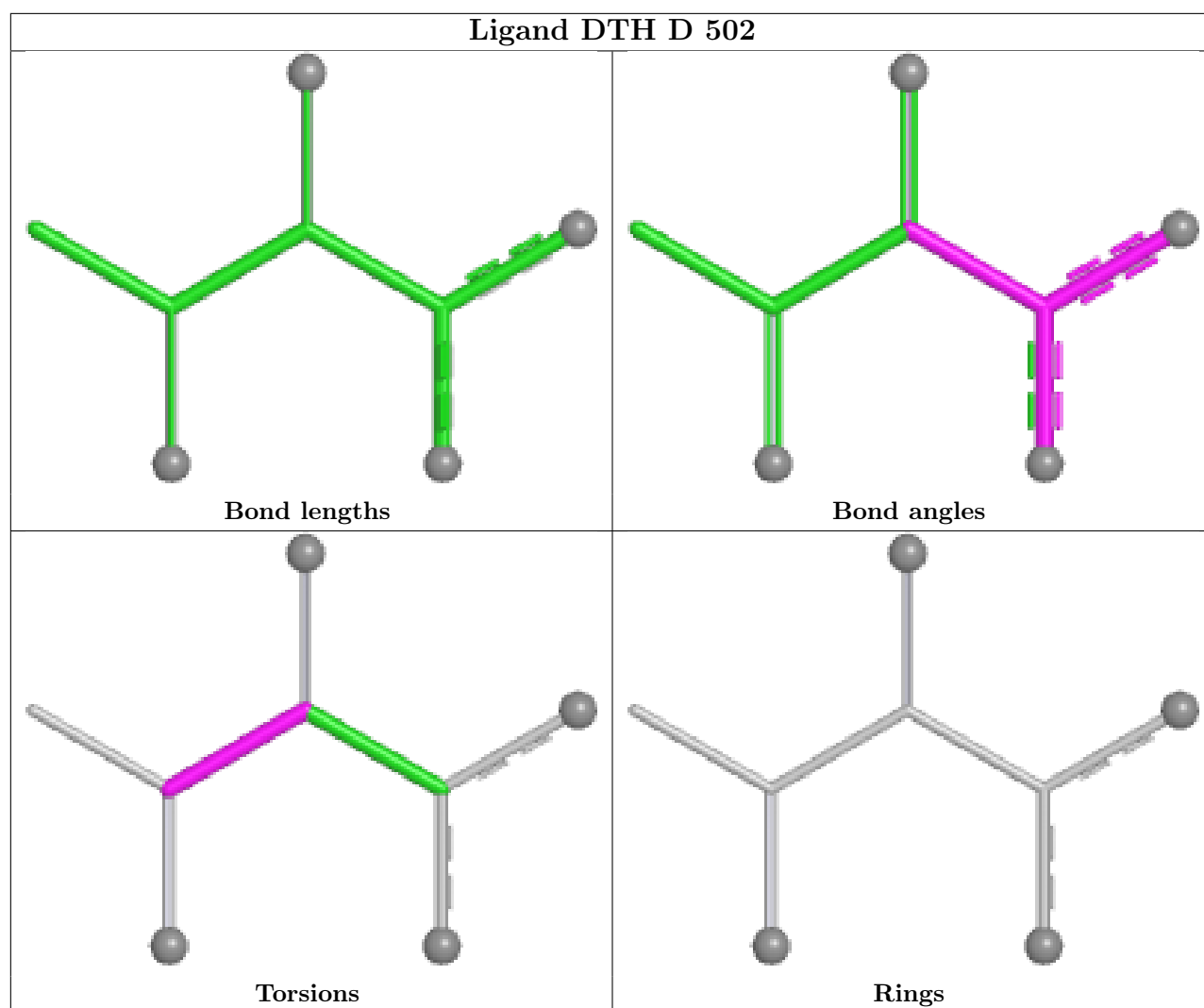
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

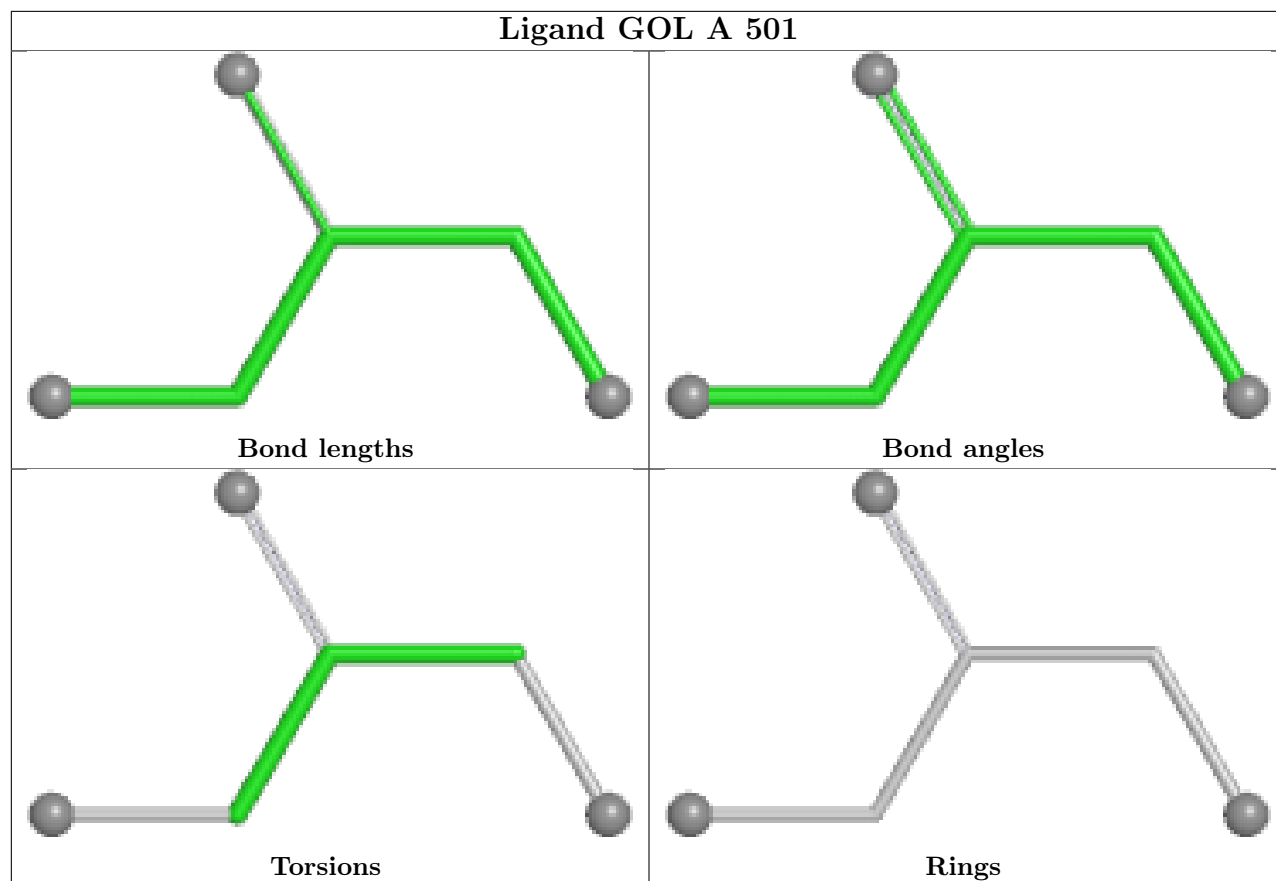


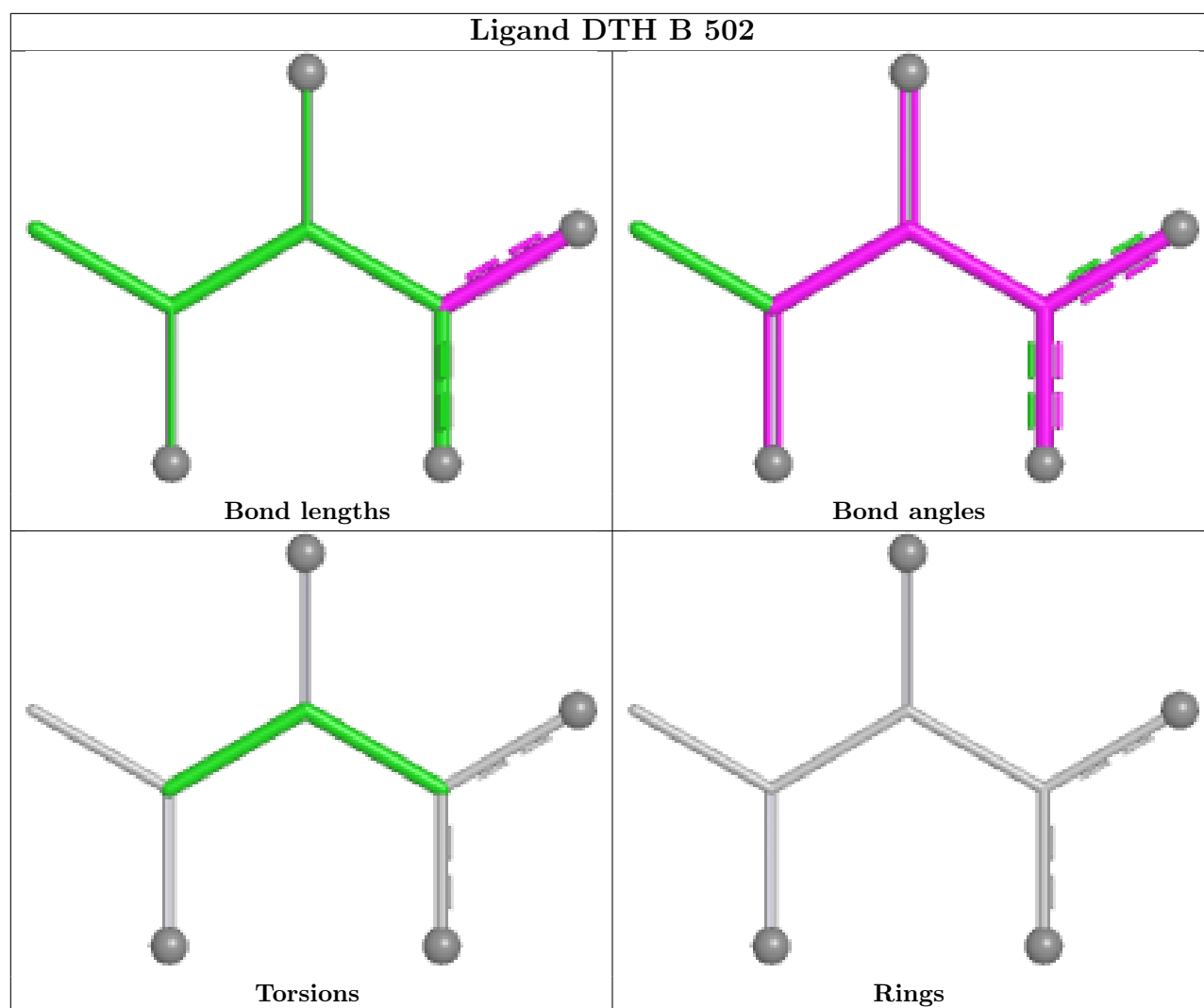












5.7 Other polymers [i](#)

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	410/416 (98%)	0.28	20 (4%) 35 41	23, 36, 60, 89	1 (0%)
1	B	410/416 (98%)	0.30	18 (4%) 39 45	23, 41, 63, 102	1 (0%)
1	C	410/416 (98%)	0.22	9 (2%) 62 69	26, 37, 55, 87	1 (0%)
1	D	410/416 (98%)	0.90	31 (7%) 20 22	35, 50, 73, 92	1 (0%)
All	All	1640/1664 (98%)	0.42	78 (4%) 35 41	23, 41, 64, 102	4 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	121	LEU	6.9
1	B	121	LEU	6.8
1	D	357	PHE	5.6
1	A	121	LEU	5.5
1	D	121	LEU	4.5
1	B	7	ASP	4.4
1	A	7	ASP	4.4
1	B	357	PHE	4.3
1	B	8	TYR	4.0
1	D	408	VAL	4.0
1	C	7	ASP	3.9
1	A	357	PHE	3.8
1	D	7	ASP	3.6
1	D	398	VAL	3.6
1	C	357	PHE	3.6
1	D	8	TYR	3.4
1	A	397	GLU	3.2
1	A	8	TYR	3.1
1	A	398	VAL	3.1
1	B	395	LYS	3.0
1	D	41	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	416	TYR	3.0
1	D	127	LEU	3.0
1	D	416	TYR	2.9
1	C	127	LEU	2.9
1	B	127	LEU	2.9
1	D	415	LEU	2.9
1	B	126	HIS	2.8
1	D	291	ILE	2.7
1	D	326	VAL	2.7
1	B	10	ALA	2.7
1	B	64	TYR	2.7
1	A	41	LYS	2.7
1	A	122	SER	2.6
1	B	398	VAL	2.6
1	B	11	PHE	2.5
1	A	407	LYS	2.5
1	C	398	VAL	2.5
1	D	221	ALA	2.5
1	D	412	ALA	2.5
1	D	393	HIS	2.4
1	D	399	LEU	2.4
1	D	9	LYS	2.4
1	B	111[A]	GLN	2.4
1	C	249	LYS	2.4
1	B	394	ASP	2.4
1	A	123	ALA	2.4
1	D	331	LYS	2.4
1	D	281	PRO	2.4
1	A	403	ARG	2.3
1	A	396	PRO	2.3
1	D	397	GLU	2.3
1	D	402	ILE	2.3
1	C	394	ASP	2.3
1	A	303	GLN	2.3
1	A	126	HIS	2.3
1	C	126	HIS	2.3
1	D	109	LEU	2.3
1	D	407	LYS	2.3
1	D	149	LYS	2.2
1	B	65	TYR	2.2
1	B	415	LEU	2.2
1	D	358	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	387	VAL	2.1
1	A	358	LYS	2.1
1	D	307	PHE	2.1
1	A	321	VAL	2.1
1	B	132	PRO	2.1
1	D	10	ALA	2.1
1	B	408	VAL	2.1
1	A	127	LEU	2.1
1	D	292	LYS	2.0
1	A	408	VAL	2.0
1	D	194	VAL	2.0
1	A	415	LEU	2.0
1	D	325	LYS	2.0
1	A	416	TYR	2.0
1	B	396	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

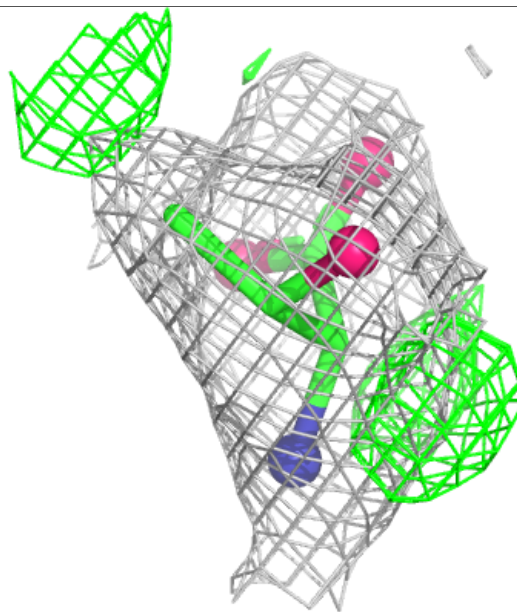
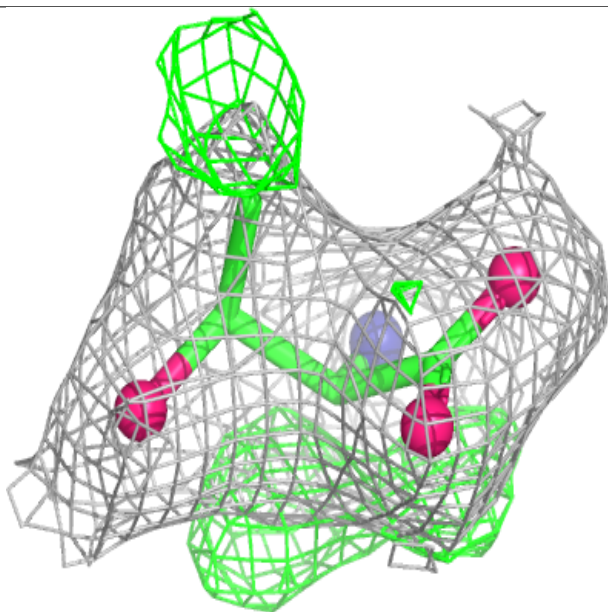
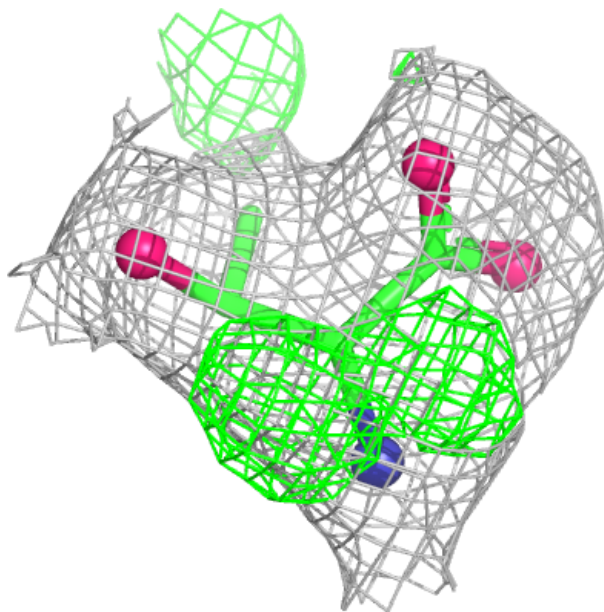
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DTH	D	502	8/8	0.86	0.18	46,64,70,72	0
3	DTH	A	502	8/8	0.92	0.14	29,52,63,67	0
3	DTH	C	502	8/8	0.92	0.14	38,51,62,71	0
2	GOL	C	501	6/6	0.92	0.14	38,43,46,82	0
3	DTH	B	502	8/8	0.93	0.13	33,59,66,74	0
4	NA	D	501	1/1	0.93	0.34	65,65,65,65	0
2	GOL	B	501	6/6	0.95	0.12	31,42,46,49	0
2	GOL	A	501	6/6	0.96	0.12	32,44,47,49	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.

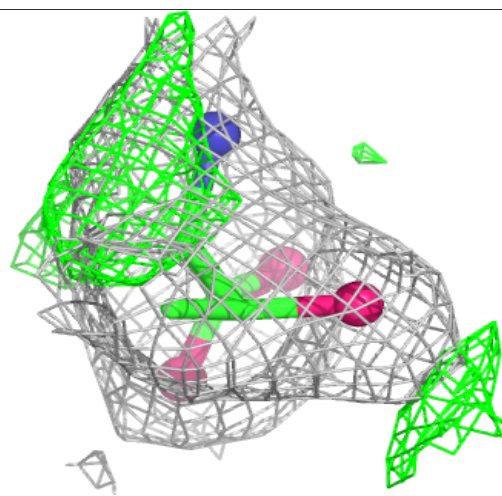
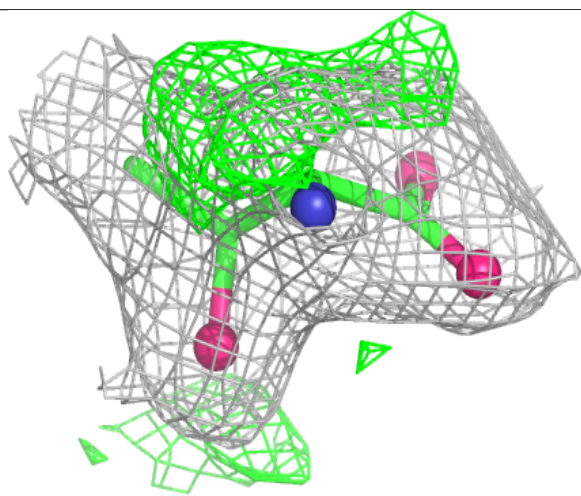
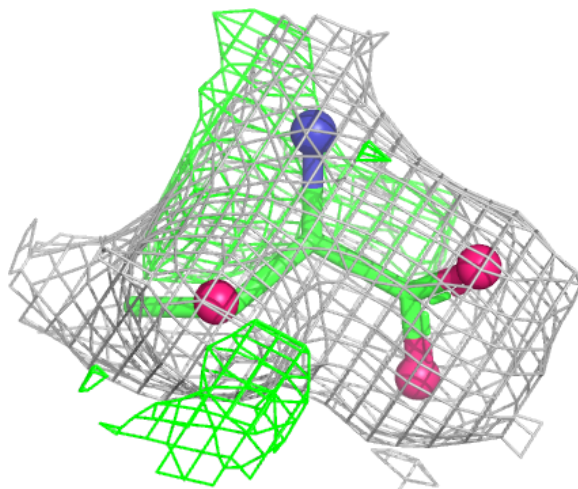
Electron density around DTH D 502:

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



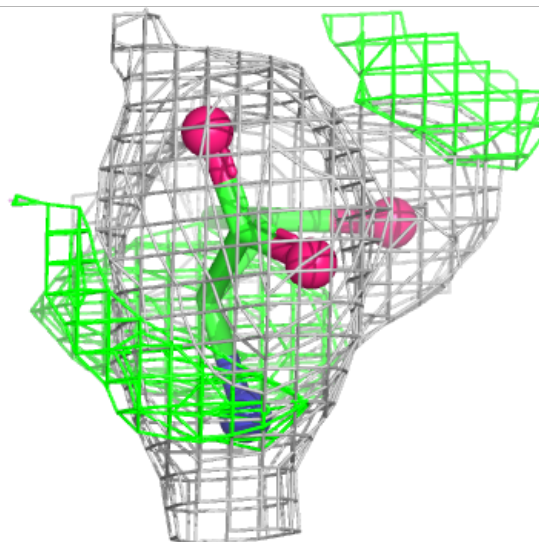
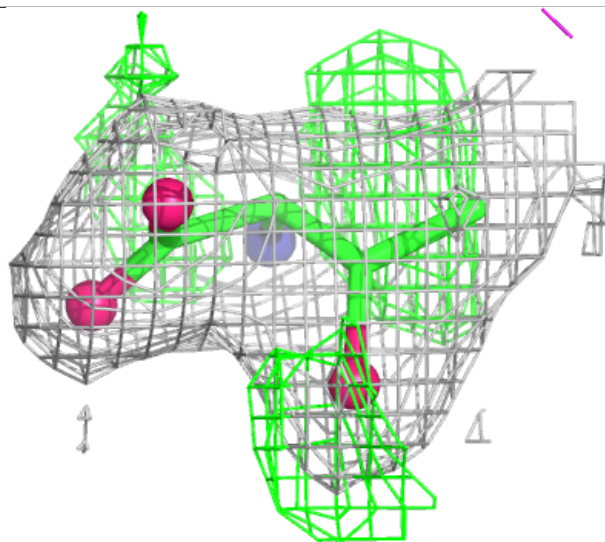
Electron density around DTH A 502:

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



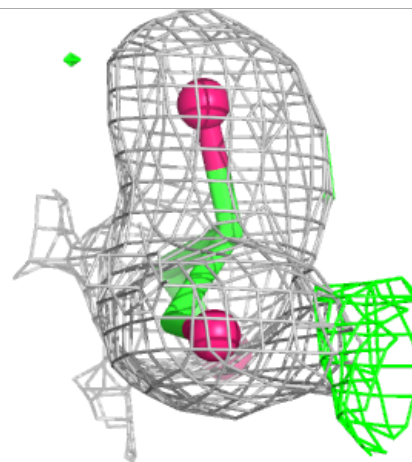
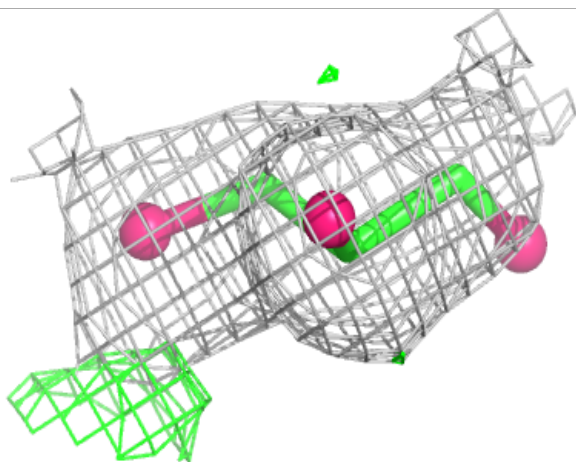
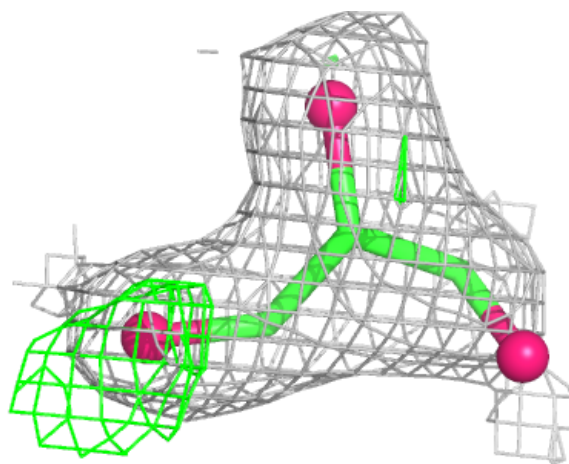
Electron density around DTH C 502:

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



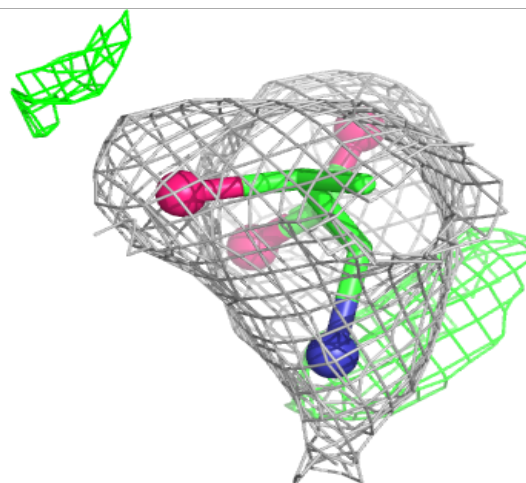
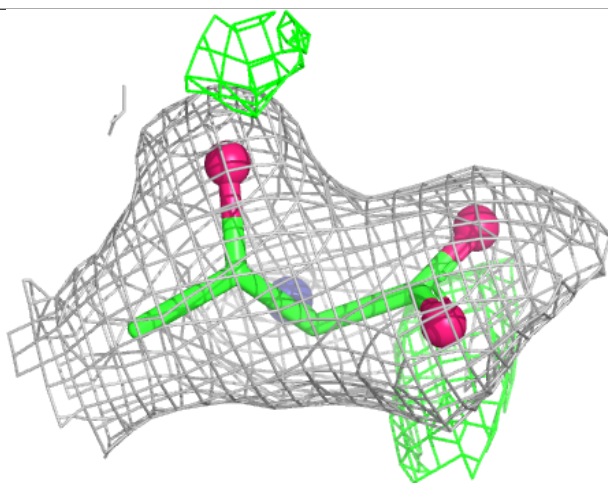
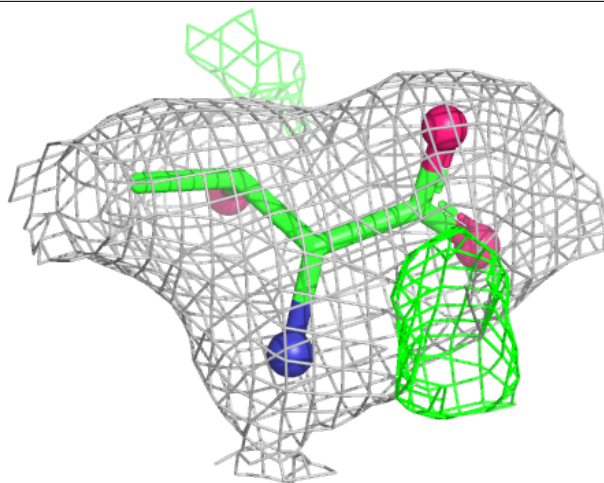
Electron density around GOL C 501:

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



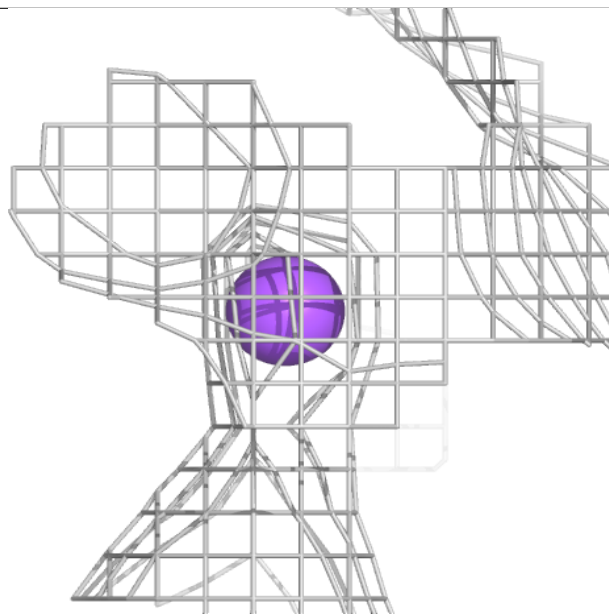
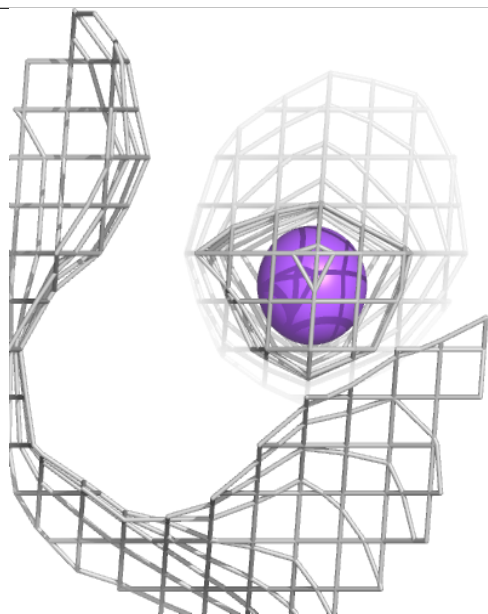
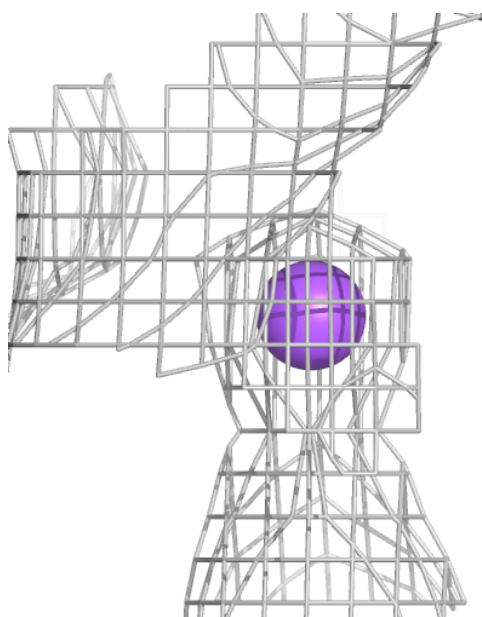
Electron density around DTH B 502:

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



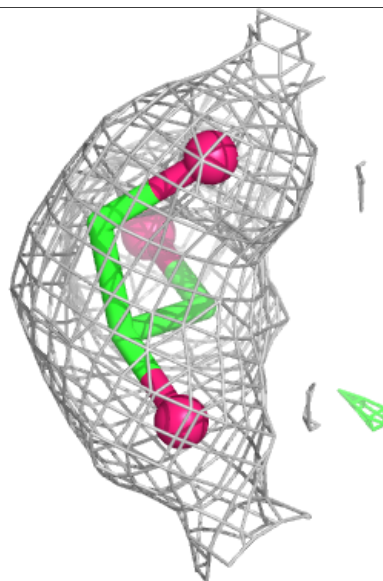
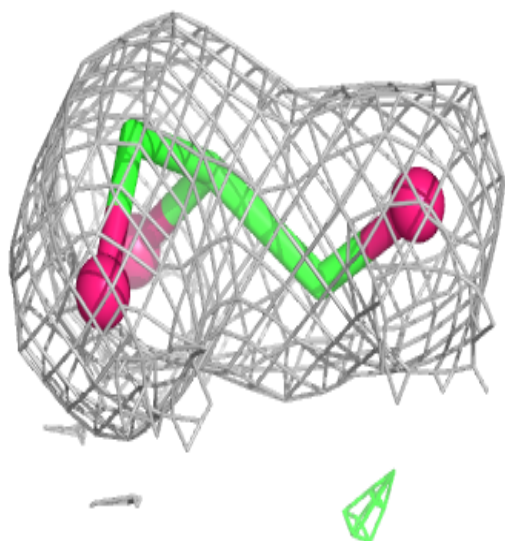
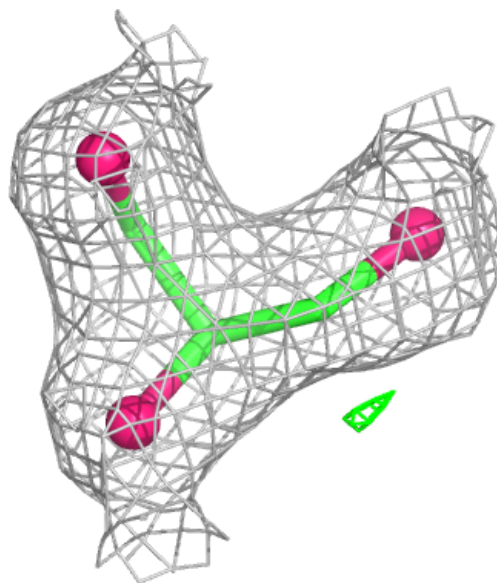
Electron density around NA D 501:

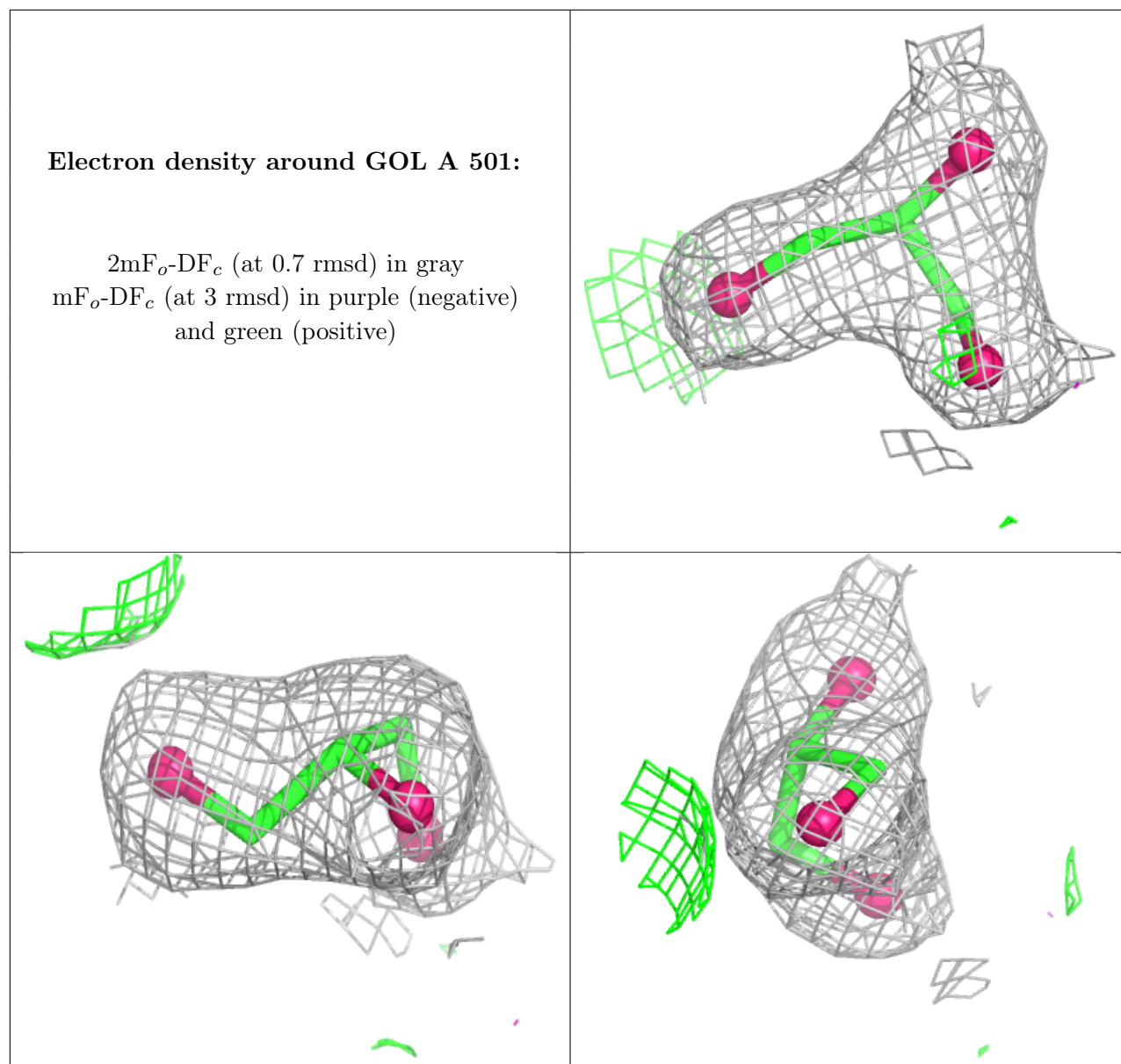
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GOL B 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.