



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:37 AM UTC

PDB ID : 9HIB / pdb_00009hib
Title : K115 acetylated human muscle pyruvate kinase, isoform M2 (PKM2)
Authors : Pavlenko, D.; Nudelman, H.; Shahar, A.; Arbely, E.
Deposited on : 2024-11-25
Resolution : 2.17 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

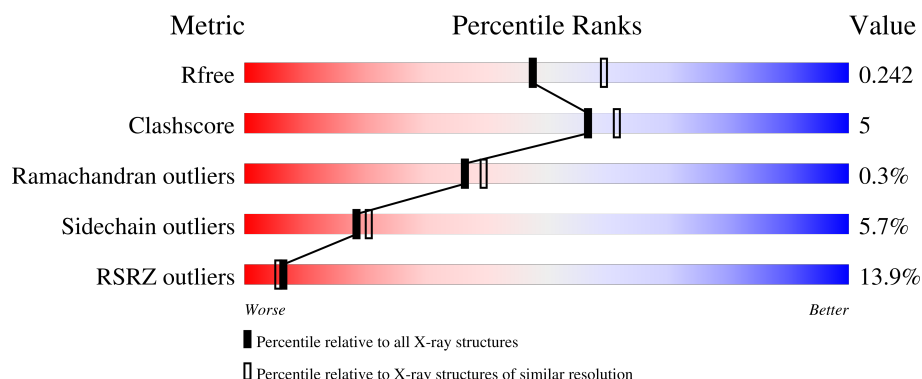
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	537	<div> <div>10%</div> <div>80%</div> <div>11%</div> <div>6%</div> </div>
1	B	537	<div> <div>8%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
1	C	537	<div> <div>5%</div> <div>81%</div> <div>11%</div> <div>6%</div> </div>
1	D	537	<div> <div>29%</div> <div>76%</div> <div>14%</div> <div>7%</div> </div>

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	TRS	C	603	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16021 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 Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	2	0
			3900	2450	699	726	25			
1	B	517	Total	C	N	O	S	0	0	0
			3968	2495	706	742	25			
1	C	513	Total	C	N	O	S	0	1	0
			3944	2481	700	737	26			
1	D	502	Total	C	N	O	S	0	0	0
			3852	2424	684	719	25			

There are 24 discrepancies between the modelled and reference sequences:

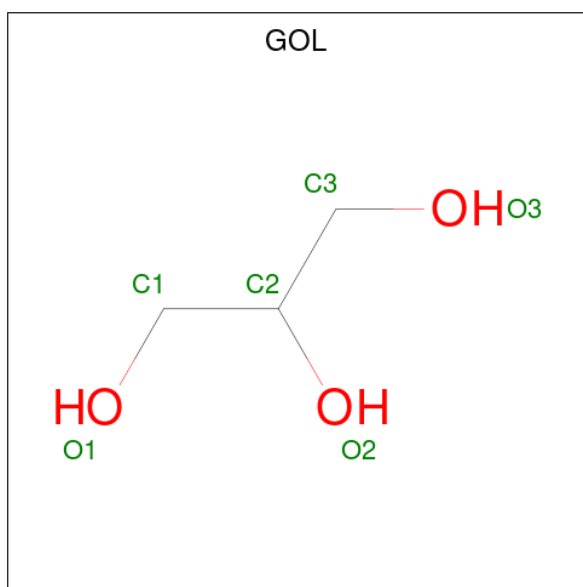
Chain	Residue	Modelled	Actual	Comment	Reference
A	532	HIS	-	expression tag	UNP P14618
A	533	HIS	-	expression tag	UNP P14618
A	534	HIS	-	expression tag	UNP P14618
A	535	HIS	-	expression tag	UNP P14618
A	536	HIS	-	expression tag	UNP P14618
A	537	HIS	-	expression tag	UNP P14618
B	532	HIS	-	expression tag	UNP P14618
B	533	HIS	-	expression tag	UNP P14618
B	534	HIS	-	expression tag	UNP P14618
B	535	HIS	-	expression tag	UNP P14618
B	536	HIS	-	expression tag	UNP P14618
B	537	HIS	-	expression tag	UNP P14618
C	532	HIS	-	expression tag	UNP P14618
C	533	HIS	-	expression tag	UNP P14618
C	534	HIS	-	expression tag	UNP P14618
C	535	HIS	-	expression tag	UNP P14618
C	536	HIS	-	expression tag	UNP P14618
C	537	HIS	-	expression tag	UNP P14618
D	532	HIS	-	expression tag	UNP P14618
D	533	HIS	-	expression tag	UNP P14618
D	534	HIS	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
D	535	HIS	-	expression tag	UNP P14618
D	536	HIS	-	expression tag	UNP P14618
D	537	HIS	-	expression tag	UNP P14618

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (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	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

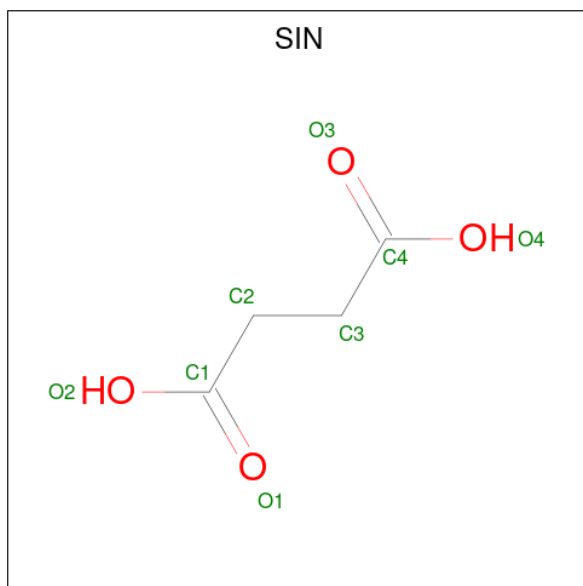
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			8	4	4		

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total K 1 1	0	0

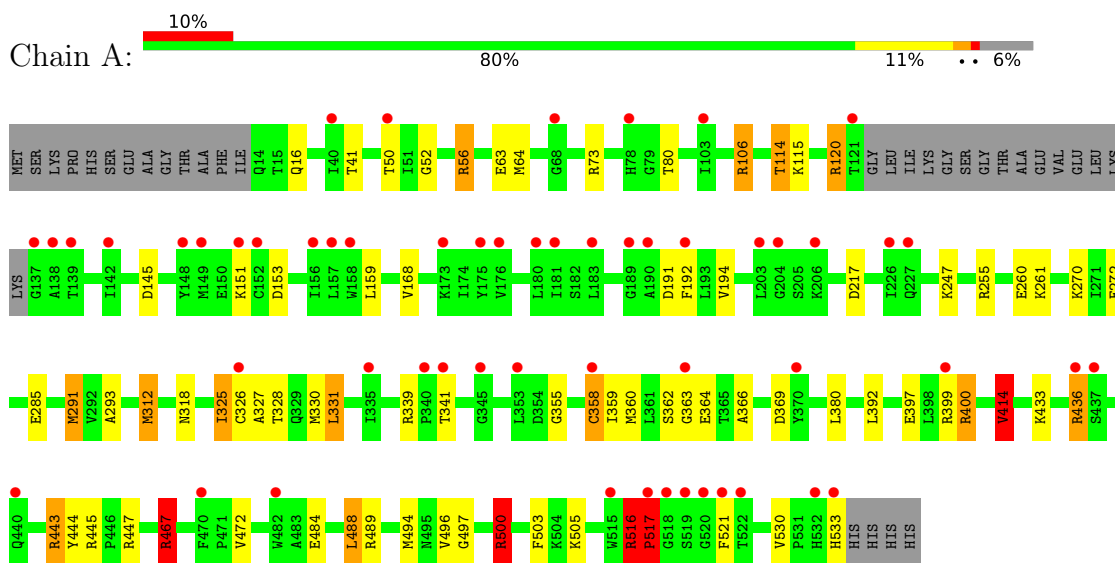
- Molecule 8 is water.

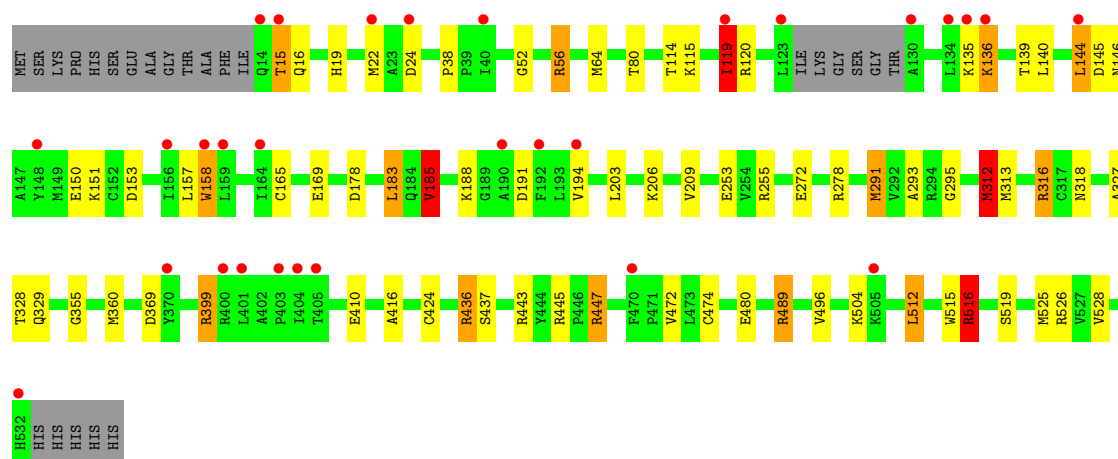
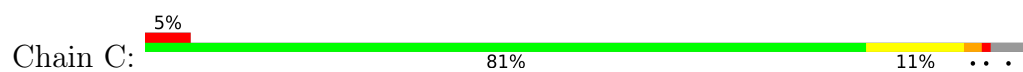
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	25	Total O 25 25	0	0
8	B	126	Total O 126 126	0	0
8	C	110	Total O 110 110	0	0
8	D	6	Total O 6 6	0	0

3 Residue-property plots [i](#)

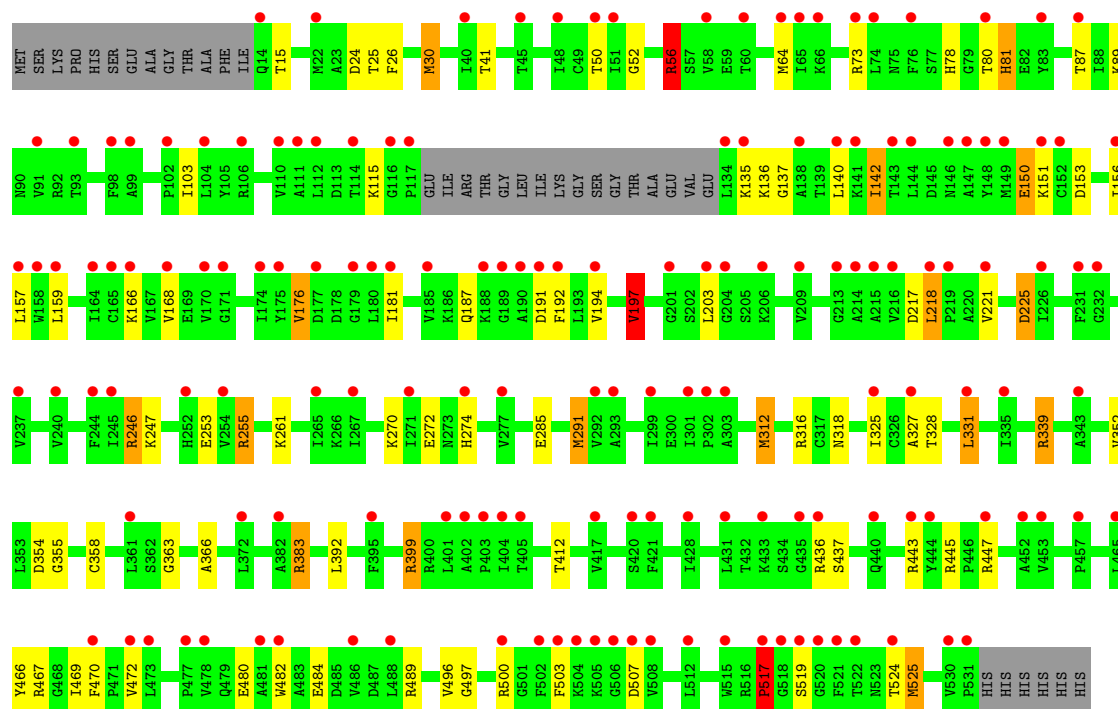
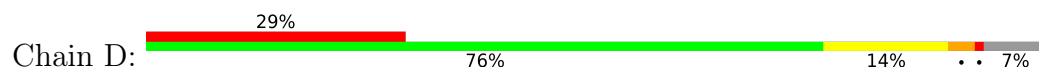
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Pyruvate kinase PKM





• Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.54Å 154.78Å 100.70Å 90.00° 107.40° 90.00°	Depositor
Resolution (Å)	81.64 – 2.17 81.64 – 2.17	Depositor EDS
% Data completeness (in resolution range)	100.0 (81.64-2.17) 100.0 (81.64-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.223 , 0.265 (Not available) , 0.242	Depositor DCC
R_{free} test set	6232 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16021	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: TRS, SIN, EDO, K, MG, GOL, ALY

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	0.75	1/3955 (0.0%)	1.40	36/5342 (0.7%)
1	B	0.92	2/4020 (0.0%)	1.38	31/5430 (0.6%)
1	C	0.89	0/3998	1.39	31/5399 (0.6%)
1	D	0.68	1/3902 (0.0%)	1.34	29/5270 (0.6%)
All	All	0.82	4/15875 (0.0%)	1.38	127/21441 (0.6%)

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	9
1	B	0	6
1	C	0	10
1	D	0	10
All	All	0	35

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	461	ARG	NE-CZ	5.66	1.39	1.33
1	A	325	ILE	C-O	-5.62	1.18	1.24
1	D	447	ARG	NE-CZ	5.20	1.38	1.33
1	B	362	SER	CA-C	5.00	1.54	1.52

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	CYS	CB-CA-C	-23.87	73.79	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	CYS	N-CA-CB	-12.29	92.83	111.64
1	A	358	CYS	N-CA-C	9.83	128.88	108.53
1	A	285	GLU	N-CA-CB	8.39	123.14	110.22
1	A	467	ARG	CG-CD-NE	-8.39	93.54	112.00
1	D	383	ARG	N-CA-CB	8.34	122.38	110.12
1	B	56	ARG	CB-CA-C	-8.20	93.20	109.67
1	B	278	ARG	CG-CD-NE	8.16	129.96	112.00
1	C	291	MET	CG-SD-CE	-8.16	82.94	100.90
1	B	447	ARG	N-CA-CB	8.01	122.14	110.20
1	A	467	ARG	CB-CA-C	-7.98	99.98	109.80
1	C	185	VAL	N-CA-CB	7.88	119.11	110.53
1	A	153	ASP	CA-CB-CG	7.84	120.44	112.60
1	B	445	ARG	NE-CZ-NH2	7.84	126.25	119.20
1	D	197	VAL	N-CA-CB	7.81	119.04	110.53
1	C	114	THR	CA-CB-OG1	-7.69	98.06	109.60
1	C	158	TRP	CB-CG-CD2	-7.53	116.25	126.80
1	B	25	THR	N-CA-CB	-7.51	97.70	111.37
1	C	525	MET	CG-SD-CE	7.44	117.27	100.90
1	A	56	ARG	CB-CA-C	-7.39	94.54	109.55
1	D	255	ARG	NE-CZ-NH1	-7.33	114.17	121.50
1	D	30	MET	CG-SD-CE	7.31	116.99	100.90
1	D	383	ARG	CB-CA-C	-7.30	98.67	110.79
1	C	445	ARG	NE-CZ-NH1	7.25	128.75	121.50
1	C	56	ARG	CB-CA-C	-7.23	95.14	109.67
1	B	185	VAL	N-CA-CB	7.23	118.41	110.53
1	A	145	ASP	CA-CB-CG	7.21	119.81	112.60
1	A	191	ASP	CA-CB-CG	7.19	119.79	112.60
1	A	106	ARG	CD-NE-CZ	7.18	134.45	124.40
1	C	158	TRP	CB-CG-CD1	7.16	137.63	126.90
1	C	191	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	467	ARG	CB-CG-CD	6.84	127.04	111.30
1	D	56	ARG	CB-CA-C	-6.84	95.91	109.67
1	B	145	ASP	CA-CB-CG	6.77	119.37	112.60
1	D	217	ASP	CB-CA-C	-6.76	96.74	109.72
1	C	410	GLU	CB-CG-CD	6.76	124.09	112.60
1	B	30	MET	CG-SD-CE	-6.69	86.19	100.90
1	D	331	LEU	N-CA-CB	-6.67	101.64	111.51
1	C	145	ASP	CA-CB-CG	6.66	119.26	112.60
1	D	253	GLU	CB-CG-CD	6.65	123.90	112.60
1	C	445	ARG	CD-NE-CZ	-6.63	115.12	124.40
1	D	274	HIS	CA-CB-CG	6.61	120.41	113.80
1	C	369	ASP	N-CA-C	-6.60	102.29	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	525	MET	CG-SD-CE	6.60	115.42	100.90
1	C	253	GLU	CB-CG-CD	6.57	123.77	112.60
1	D	225	ASP	CA-CB-CG	6.54	119.14	112.60
1	B	191	ASP	CA-CB-CG	6.51	119.11	112.60
1	C	480	GLU	CB-CG-CD	6.50	123.66	112.60
1	C	64	MET	CG-SD-CE	-6.49	86.62	100.90
1	B	254	VAL	N-CA-CB	6.36	117.99	110.55
1	B	80	THR	CA-CB-OG1	-6.35	100.08	109.60
1	A	64	MET	CG-SD-CE	-6.34	86.95	100.90
1	A	80	THR	CA-CB-OG1	-6.32	100.11	109.60
1	C	15	THR	CA-CB-OG1	-6.25	100.22	109.60
1	A	312	MET	CG-SD-CE	-6.21	87.24	100.90
1	B	25	THR	OG1-CB-CG2	6.18	121.67	109.30
1	C	153	ASP	CA-CB-CG	6.13	118.73	112.60
1	B	410	GLU	CB-CG-CD	6.08	122.94	112.60
1	D	153	ASP	CA-CB-CG	6.08	118.67	112.60
1	A	106	ARG	CG-CD-NE	6.07	125.35	112.00
1	B	64	MET	CG-SD-CE	-6.06	87.56	100.90
1	B	456	ASN	CB-CA-C	6.05	117.04	110.08
1	D	470	PHE	CB-CA-C	5.97	115.81	110.44
1	A	445	ARG	NE-CZ-NH2	5.96	124.57	119.20
1	A	362	SER	CA-C-N	-5.94	117.00	123.30
1	A	362	SER	C-N-CA	-5.94	117.00	123.30
1	C	272	GLU	CB-CA-C	-5.94	99.77	110.35
1	D	192	PHE	CA-CB-CG	5.92	119.72	113.80
1	D	81	HIS	CB-CG-CD2	5.92	138.89	131.20
1	D	291	MET	CG-SD-CE	-5.87	87.98	100.90
1	C	145	ASP	CB-CA-C	5.84	119.03	110.26
1	A	369	ASP	N-CA-C	-5.84	103.23	110.41
1	D	217	ASP	CA-CB-CG	5.83	118.43	112.60
1	C	19	HIS	CB-CA-C	5.77	119.93	110.88
1	C	399	ARG	CB-CA-C	5.70	120.53	110.85
1	B	436	ARG	CB-CG-CD	5.69	124.38	111.30
1	D	191	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	516	ARG	CA-C-N	5.67	126.93	119.84
1	A	516	ARG	C-N-CA	5.67	126.93	119.84
1	A	120	ARG	CA-C-N	5.64	131.86	121.70
1	A	120	ARG	C-N-CA	5.64	131.86	121.70
1	A	192	PHE	CA-CB-CG	5.61	119.41	113.80
1	B	123	LEU	CA-C-N	5.59	131.76	121.70
1	B	123	LEU	C-N-CA	5.59	131.76	121.70
1	A	414	VAL	N-CA-CB	5.58	118.95	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	LYS	CA-CB-CG	5.55	125.20	114.10
1	C	329	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	B	396	GLU	CB-CG-CD	5.54	122.02	112.60
1	D	399	ARG	CB-CA-C	-5.53	102.20	110.88
1	C	139	THR	CA-CB-OG1	-5.52	101.32	109.60
1	B	192	PHE	CA-CB-CG	5.50	119.30	113.80
1	D	64	MET	CG-SD-CE	-5.50	88.81	100.90
1	B	86	GLU	CG-CD-OE2	-5.49	105.78	118.40
1	C	436	ARG	NE-CZ-NH2	-5.47	114.27	119.20
1	C	369	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	29	HIS	CB-CG-ND1	-5.45	114.53	122.70
1	A	261	LYS	N-CA-CB	5.43	118.10	110.12
1	B	256	LYS	CG-CD-CE	5.37	123.64	111.30
1	A	400	ARG	CA-CB-CG	5.36	124.82	114.10
1	C	312	MET	CG-SD-CE	5.34	112.66	100.90
1	B	532	HIS	CA-CB-CG	5.33	119.13	113.80
1	C	80	THR	CA-CB-OG1	-5.31	101.63	109.60
1	C	119	ILE	CB-CA-C	5.28	118.70	110.83
1	A	63	GLU	CA-C-N	5.26	127.64	120.54
1	A	63	GLU	C-N-CA	5.26	127.64	120.54
1	A	114	THR	N-CA-CB	-5.23	102.61	111.50
1	D	24	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	436	ARG	CD-NE-CZ	5.22	131.70	124.40
1	B	114	THR	OG1-CB-CG2	5.21	119.73	109.30
1	B	241	PHE	CA-CB-CG	5.21	119.02	113.80
1	D	339	ARG	CG-CD-NE	5.21	123.47	112.00
1	D	354	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	169	GLU	CB-CG-CD	5.18	121.42	112.60
1	D	517	PRO	N-CA-C	5.17	123.12	112.47
1	B	517	PRO	N-CA-C	5.17	121.45	113.75
1	D	261	LYS	CB-CA-C	-5.15	101.92	110.68
1	A	217	ASP	CA-CB-CG	5.14	117.75	112.60
1	D	312	MET	CG-SD-CE	-5.11	89.67	100.90
1	A	291	MET	CG-SD-CE	-5.10	89.68	100.90
1	D	507	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	114	THR	CA-CB-CG2	5.06	119.10	110.50
1	B	29	HIS	CB-CG-CD2	5.05	137.77	131.20
1	D	255	ARG	CD-NE-CZ	5.04	131.46	124.40
1	B	133	GLU	CB-CG-CD	5.02	121.14	112.60
1	B	521	PHE	N-CA-CB	-5.02	102.91	111.20
1	C	22	MET	CG-SD-CE	5.01	111.93	100.90
1	C	136	LYS	CB-CA-C	5.01	117.03	110.06

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ARG	Sidechain
1	A	255	ARG	Sidechain
1	A	339	ARG	Sidechain
1	A	399	ARG	Sidechain
1	A	436	ARG	Sidechain
1	A	443	ARG	Sidechain
1	A	467	ARG	Sidechain
1	A	489	ARG	Sidechain
1	A	500	ARG	Sidechain
1	B	106	ARG	Sidechain
1	B	120	ARG	Sidechain
1	B	339	ARG	Sidechain
1	B	400	ARG	Sidechain
1	B	455	ARG	Sidechain
1	B	92	ARG	Sidechain
1	C	120	ARG	Sidechain
1	C	255	ARG	Sidechain
1	C	278	ARG	Sidechain
1	C	316	ARG	Sidechain
1	C	436	ARG	Sidechain
1	C	443	ARG	Sidechain
1	C	447	ARG	Sidechain
1	C	489	ARG	Sidechain
1	C	516	ARG	Sidechain
1	C	526	ARG	Sidechain
1	D	255	ARG	Sidechain
1	D	316	ARG	Sidechain
1	D	327	ALA	Peptide
1	D	339	ARG	Sidechain
1	D	383	ARG	Sidechain
1	D	399	ARG	Sidechain
1	D	436	ARG	Sidechain
1	D	445	ARG	Sidechain
1	D	489	ARG	Sidechain
1	D	56	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	3900	0	3967	46	0
1	B	3968	0	4042	24	0
1	C	3944	0	4022	44	0
1	D	3852	0	3929	31	0
2	A	6	0	8	1	0
2	B	6	0	8	0	0
2	C	18	0	24	4	0
2	D	6	0	8	0	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
3	C	16	0	24	2	0
3	D	4	0	6	0	0
4	B	1	0	0	0	0
5	C	8	0	12	3	0
6	C	8	0	4	1	0
7	C	1	0	0	0	0
8	A	25	0	0	0	0
8	B	126	0	0	1	0
8	C	110	0	0	3	0
8	D	6	0	0	0	0
All	All	16021	0	16078	145	0

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

All (145) 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:325:ILE:HA	1:A:358:CYS:SG	2.06	0.94
1:C:312:MET:HE2	1:C:313:MET:CA	2.01	0.89
1:B:25:THR:HG22	1:B:28:GLU:H	1.38	0.89
1:C:437:SER:OG	2:C:608:GOL:H31	1.73	0.88
1:B:43:ARG:HH22	1:B:70:ASN:HD21	1.17	0.88
1:A:494:MET:HE1	1:A:530:VAL:HG22	1.55	0.86
1:B:474:CYS:SG	8:B:745:HOH:O	2.35	0.84
1:C:312:MET:HE2	1:C:313:MET:HA	1.59	0.84
1:C:312:MET:HE2	1:C:313:MET:N	1.94	0.83
1:A:50:THR:CG2	1:A:73:ARG:HH11	1.94	0.81
1:A:50:THR:HG21	1:A:73:ARG:HH11	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:ARG:HH11	1:A:500:ARG:HG3	1.47	0.79
1:C:15:THR:O	1:C:38:PRO:O	2.00	0.79
1:D:50:THR:CG2	1:D:73:ARG:HH11	1.95	0.79
1:D:50:THR:HG21	1:D:73:ARG:HH11	1.50	0.77
1:A:326:CYS:SG	1:A:359:ILE:HA	2.25	0.76
1:C:291:MET:CE	1:C:293:ALA:HB2	2.15	0.76
1:C:312:MET:CE	1:C:313:MET:HA	2.17	0.74
1:A:447[A]:ARG:HG3	1:A:447[A]:ARG:HH21	1.52	0.74
1:A:494:MET:HE2	1:A:530:VAL:HG13	1.70	0.73
1:C:119:ILE:HG12	1:C:209:VAL:HB	1.69	0.73
1:C:519:SER:HA	2:C:608:GOL:H2	1.69	0.72
1:A:326:CYS:N	1:A:358:CYS:SG	2.61	0.70
1:B:47:ILE:H	1:B:70:ASN:HD22	1.38	0.70
1:C:474:CYS:SG	8:C:762:HOH:O	2.49	0.69
1:C:144:LEU:O	1:C:158:TRP:HH2	1.79	0.65
1:C:515:TRP:CE3	1:C:516:ARG:HB2	2.38	0.59
1:C:15:THR:HG23	1:C:16:GLN:HG3	1.84	0.59
5:C:603:TRS:H21	3:C:609:EDO:O1	2.04	0.58
1:C:312:MET:HE2	1:C:312:MET:C	2.27	0.58
1:A:325:ILE:HA	1:A:358:CYS:CB	2.33	0.58
1:A:330:MET:O	1:A:364:GLU:OE2	2.21	0.58
1:A:50:THR:HG21	1:A:73:ARG:NH1	2.18	0.57
1:C:144:LEU:C	1:C:158:TRP:CH2	2.82	0.57
1:B:339:ARG:NH2	1:C:178:ASP:O	2.37	0.56
1:C:312:MET:HE1	1:C:313:MET:HG2	1.86	0.56
1:A:50:THR:HG22	1:A:73:ARG:HD3	1.89	0.55
1:B:255:ARG:CZ	1:B:267:ILE:HD12	2.37	0.55
1:B:121:THR:HG23	1:B:157:LEU:HD11	1.87	0.55
1:A:325:ILE:CA	1:A:358:CYS:SG	2.90	0.54
1:B:103:ILE:O	1:B:500:ARG:NH1	2.40	0.54
1:A:447[A]:ARG:HG3	1:A:447[A]:ARG:NH2	2.20	0.53
1:C:291:MET:HE3	1:C:293:ALA:HA	1.90	0.53
1:D:103:ILE:O	1:D:500:ARG:NH1	2.41	0.53
1:C:144:LEU:C	1:C:158:TRP:HH2	2.17	0.52
1:C:318:ASN:HD21	1:C:355:GLY:HA3	1.74	0.52
1:A:488:LEU:HD12	1:A:488:LEU:O	2.10	0.52
1:D:56:ARG:HE	1:D:87:THR:HG22	1.75	0.52
1:B:43:ARG:HH22	1:B:70:ASN:ND2	1.98	0.52
1:D:50:THR:HG21	1:D:73:ARG:NH1	2.22	0.52
1:B:52:GLY:O	1:B:56:ARG:HG3	2.11	0.51
1:A:447[A]:ARG:NH2	1:A:447[A]:ARG:CG	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:ASN:HD21	1:D:355:GLY:HA3	1.75	0.51
1:A:50:THR:HG22	1:A:73:ARG:HH11	1.75	0.51
1:D:137:GLY:O	1:D:197:VAL:HG13	2.10	0.51
1:C:158:TRP:CE3	1:C:158:TRP:HA	2.46	0.51
1:A:318:ASN:HD21	1:A:355:GLY:HA3	1.75	0.51
1:C:472:VAL:HG11	1:C:496:VAL:HG11	1.93	0.50
1:C:291:MET:HE3	1:C:293:ALA:CA	2.41	0.50
1:B:318:ASN:HD21	1:B:355:GLY:HA3	1.75	0.50
1:C:312:MET:CE	1:C:313:MET:HG2	2.42	0.50
1:D:363:GLY:HA2	1:D:366:ALA:HB3	1.93	0.49
1:D:140:LEU:HD21	1:D:142:ILE:HG12	1.94	0.49
1:A:270:LYS:HE3	1:A:291:MET:HE1	1.94	0.49
1:A:293:ALA:HB1	2:A:600:GOL:H31	1.94	0.49
1:D:56:ARG:NE	1:D:87:THR:HG22	2.28	0.49
1:A:327:ALA:HB1	1:A:360:MET:HE2	1.95	0.49
5:C:603:TRS:H32	8:C:701:HOH:O	2.12	0.49
1:C:312:MET:HE3	1:C:316:ARG:HD2	1.95	0.48
1:D:26:PHE:CE2	1:D:30:MET:HE2	2.48	0.48
1:D:218:LEU:O	1:D:246:ARG:NH2	2.46	0.48
1:A:516:ARG:HG3	1:A:517:PRO:HD2	1.94	0.48
1:C:291:MET:CE	1:C:293:ALA:CB	2.90	0.48
1:D:50:THR:HG22	1:D:73:ARG:HH11	1.75	0.48
1:D:150:GLU:HB3	1:D:157:LEU:HD21	1.95	0.48
1:A:363:GLY:HA2	1:A:366:ALA:HB3	1.95	0.48
1:A:325:ILE:HG23	1:A:358:CYS:HB2	1.96	0.47
1:B:455:ARG:HH22	1:B:485:ASP:CG	2.22	0.47
1:D:80:THR:OG1	1:D:81:HIS:N	2.46	0.47
1:D:482:TRP:CZ3	1:D:517:PRO:HA	2.49	0.47
1:D:270:LYS:HE3	1:D:291:MET:HE1	1.97	0.47
1:A:326:CYS:SG	1:A:326:CYS:O	2.72	0.47
1:A:291:MET:HE2	1:A:293:ALA:HB2	1.96	0.46
1:B:47:ILE:H	1:B:70:ASN:ND2	2.12	0.46
1:C:144:LEU:O	1:C:158:TRP:CH2	2.66	0.46
1:A:414:VAL:HG22	1:A:444:TYR:CE2	2.51	0.45
1:C:291:MET:HE3	1:C:293:ALA:CB	2.46	0.45
1:C:146:ASN:OD1	1:C:158:TRP:CZ2	2.70	0.45
1:B:121:THR:CG2	1:B:157:LEU:HD11	2.47	0.45
1:C:140:LEU:HD23	1:C:183:LEU:HD21	1.97	0.45
1:A:397:GLU:CD	1:D:25:THR:HB	2.42	0.45
1:A:494:MET:CE	1:A:530:VAL:HG22	2.37	0.45
1:C:416:ALA:HB2	1:C:512:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:VAL:HG11	1:B:496:VAL:HG11	2.00	0.44
1:C:447:ARG:HD2	8:C:774:HOH:O	2.17	0.44
6:C:606:SIN:H22	2:C:607:GOL:H12	2.00	0.44
1:A:516:ARG:HB2	1:A:516:ARG:HH11	1.82	0.44
1:B:494:MET:HG2	1:B:531:PRO:HD2	1.99	0.44
1:A:447[A]:ARG:HH21	1:A:447[A]:ARG:CG	2.17	0.44
1:A:516:ARG:HH11	1:A:516:ARG:CB	2.30	0.44
1:C:327:ALA:HB1	1:C:360:MET:HE2	1.99	0.44
1:C:52:GLY:O	1:C:56:ARG:HG3	2.18	0.44
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.98	0.44
1:A:358:CYS:O	1:A:359:ILE:C	2.58	0.43
1:A:447[B]:ARG:HH11	1:A:447[B]:ARG:HD2	1.48	0.43
1:B:416:ALA:HB2	1:B:512:LEU:HD21	1.99	0.43
1:B:138:ALA:O	1:B:197:VAL:HG12	2.17	0.43
1:C:312:MET:HE2	1:C:313:MET:CG	2.49	0.43
1:D:325:ILE:HD12	1:D:358:CYS:HB2	2.00	0.43
1:A:16:GLN:O	1:A:447[B]:ARG:NH2	2.52	0.43
1:D:176:VAL:HG13	1:D:181:ILE:HB	2.01	0.43
1:A:472:VAL:HG11	1:A:496:VAL:HG11	2.01	0.43
1:A:494:MET:HE3	1:A:494:MET:HA	2.01	0.43
1:B:327:ALA:HB1	1:B:360:MET:HE2	2.01	0.42
1:C:312:MET:CE	1:C:312:MET:C	2.92	0.42
1:A:414:VAL:HG22	1:A:444:TYR:CZ	2.55	0.42
1:D:50:THR:HG22	1:D:73:ARG:HD3	2.01	0.42
1:A:494:MET:CE	1:A:530:VAL:HG13	2.43	0.42
1:D:52:GLY:O	1:D:56:ARG:HG3	2.18	0.42
1:D:221:VAL:HG13	1:D:225:ASP:HB2	2.02	0.42
1:D:26:PHE:CD2	1:D:30:MET:HE2	2.55	0.42
1:C:157:LEU:HD13	1:C:203:LEU:HD21	2.02	0.42
1:A:400:ARG:HH12	1:C:24:ASP:HA	1.85	0.41
1:C:183:LEU:HD12	1:C:183:LEU:N	2.35	0.41
1:A:52:GLY:O	1:A:56:ARG:HG3	2.20	0.41
1:B:527:VAL:CG1	1:D:412:THR:OG1	2.68	0.41
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.55	0.41
1:D:221:VAL:HG13	1:D:225:ASP:CB	2.50	0.41
1:D:472:VAL:HG11	1:D:496:VAL:HG11	2.03	0.41
1:C:169:GLU:O	1:C:185:VAL:HG22	2.21	0.41
1:A:330:MET:O	1:A:331:LEU:HB2	2.20	0.41
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.56	0.41
1:C:146:ASN:OD1	1:C:158:TRP:HZ2	2.02	0.41
5:C:603:TRS:H11	2:C:608:GOL:H32	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:LEU:HD12	1:A:488:LEU:C	2.46	0.41
1:B:445:ARG:HH11	1:B:445:ARG:HD2	1.61	0.41
1:C:489:ARG:NH1	3:C:609:EDO:O2	2.50	0.41
1:D:352:VAL:HG13	1:D:467:ARG:HH22	1.86	0.41
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.56	0.40
1:B:274:HIS:HD2	1:B:278:ARG:HH12	1.69	0.40
1:D:392:LEU:O	1:D:392:LEU:HD23	2.21	0.40
1:C:165:CYS:O	1:C:188:LYS:NZ	2.54	0.40
1:C:169:GLU:HA	1:C:188:LYS:HE2	2.04	0.40
1:A:326:CYS:SG	1:A:359:ILE:HG22	2.62	0.40
1:B:157:LEU:HD13	1:B:203:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/537 (94%)	488 (97%)	12 (2%)	2 (0%)	30	31
1	B	512/537 (95%)	503 (98%)	8 (2%)	1 (0%)	43	49
1	C	509/537 (95%)	500 (98%)	7 (1%)	2 (0%)	30	31
1	D	497/537 (93%)	479 (96%)	16 (3%)	2 (0%)	30	31
All	All	2020/2148 (94%)	1970 (98%)	43 (2%)	7 (0%)	36	39

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	517	PRO
1	D	328	THR
1	B	328	THR
1	A	328	THR

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Mol	Chain	Res	Type
1	C	328	THR
1	D	159	LEU
1	C	295	GLY

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	418/441 (95%)	391 (94%)	27 (6%)	15	16
1	B	425/441 (96%)	405 (95%)	20 (5%)	23	28
1	C	423/441 (96%)	406 (96%)	17 (4%)	28	35
1	D	413/441 (94%)	381 (92%)	32 (8%)	12	12
All	All	1679/1764 (95%)	1583 (94%)	96 (6%)	18	20

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	106	ARG
1	A	114	THR
1	A	151	LYS
1	A	159	LEU
1	A	168	VAL
1	A	194	VAL
1	A	247	LYS
1	A	260	GLU
1	A	272	GLU
1	A	312	MET
1	A	331	LEU
1	A	341	THR
1	A	380	LEU
1	A	392	LEU
1	A	414	VAL
1	A	433	LYS
1	A	443	ARG

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Mol	Chain	Res	Type
1	A	467	ARG
1	A	484	GLU
1	A	488	LEU
1	A	500	ARG
1	A	505	LYS
1	A	516	ARG
1	A	517	PRO
1	A	521	PHE
1	A	533	HIS
1	B	25	THR
1	B	120	ARG
1	B	156	ILE
1	B	168	VAL
1	B	180	LEU
1	B	185	VAL
1	B	191	ASP
1	B	193	LEU
1	B	194	VAL
1	B	197	VAL
1	B	261	LYS
1	B	272	GLU
1	B	331	LEU
1	B	424	CYS
1	B	443	ARG
1	B	447	ARG
1	B	455	ARG
1	B	500	ARG
1	B	519	SER
1	B	527	VAL
1	C	119	ILE
1	C	135	LYS
1	C	136	LYS
1	C	144	LEU
1	C	150	GLU
1	C	151	LYS
1	C	183	LEU
1	C	185	VAL
1	C	194	VAL
1	C	206	LYS
1	C	312	MET
1	C	399	ARG
1	C	424	CYS

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Mol	Chain	Res	Type
1	C	504	LYS
1	C	512	LEU
1	C	516	ARG
1	C	528	VAL
1	D	15	THR
1	D	41	THR
1	D	78	HIS
1	D	89	LYS
1	D	135	LYS
1	D	136	LYS
1	D	142	ILE
1	D	150	GLU
1	D	151	LYS
1	D	156	ILE
1	D	166	LYS
1	D	168	VAL
1	D	176	VAL
1	D	187	GLN
1	D	194	VAL
1	D	197	VAL
1	D	203	LEU
1	D	218	LEU
1	D	246	ARG
1	D	247	LYS
1	D	272	GLU
1	D	285	GLU
1	D	312	MET
1	D	331	LEU
1	D	437	SER
1	D	443	ARG
1	D	480	GLU
1	D	484	GLU
1	D	517	PRO
1	D	519	SER
1	D	524	THR
1	D	525	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	318	ASN

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Mol	Chain	Res	Type
1	A	393	GLN
1	A	479	GLN
1	B	29	HIS
1	B	70	ASN
1	B	252	HIS
1	B	318	ASN
1	B	393	GLN
1	B	479	GLN
1	B	532	HIS
1	C	44	ASN
1	C	146	ASN
1	C	252	HIS
1	C	318	ASN
1	C	393	GLN
1	C	479	GLN
1	D	16	GLN
1	D	146	ASN
1	D	274	HIS
1	D	318	ASN
1	D	391	HIS
1	D	393	GLN
1	D	479	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	ALY	D	115	1	10,11,12	0.51	0	7,12,14	1.60	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	ALY	A	115	1	10,11,12	0.71	0	7,12,14	1.50	2 (28%)
1	ALY	B	115	1	10,11,12	0.57	0	7,12,14	1.63	1 (14%)
1	ALY	C	115	1	10,11,12	0.51	0	7,12,14	1.30	1 (14%)

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
1	ALY	D	115	1	-	6/9/10/12	-
1	ALY	A	115	1	-	6/9/10/12	-
1	ALY	B	115	1	-	5/9/10/12	-
1	ALY	C	115	1	-	4/9/10/12	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	ALY	CE-NZ-CH	3.61	127.89	122.56
1	C	115	ALY	CE-NZ-CH	3.21	127.30	122.56
1	D	115	ALY	CE-NZ-CH	2.86	126.78	122.56
1	A	115	ALY	CE-NZ-CH	2.49	126.24	122.56
1	D	115	ALY	CH3-CH-NZ	2.15	119.79	116.12
1	A	115	ALY	CH3-CH-NZ	2.11	119.72	116.12

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	115	ALY	CH3-CH-NZ-CE
1	A	115	ALY	N-CA-CB-CG
1	A	115	ALY	C-CA-CB-CG
1	C	115	ALY	OH-CH-NZ-CE
1	C	115	ALY	CH3-CH-NZ-CE
1	D	115	ALY	N-CA-CB-CG
1	D	115	ALY	C-CA-CB-CG
1	A	115	ALY	OH-CH-NZ-CE
1	B	115	ALY	OH-CH-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	B	115	ALY	CH3-CH-NZ-CE
1	D	115	ALY	OH-CH-NZ-CE
1	D	115	ALY	CH3-CH-NZ-CE
1	C	115	ALY	CG-CD-CE-NZ
1	A	115	ALY	CE-CD-CG-CB
1	A	115	ALY	CA-CB-CG-CD
1	D	115	ALY	CA-CB-CG-CD
1	D	115	ALY	CG-CD-CE-NZ
1	B	115	ALY	CA-CB-CG-CD
1	B	115	ALY	C-CA-CB-CG
1	C	115	ALY	C-CA-CB-CG
1	B	115	ALY	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	A	600	-	5,5,5	0.18	0	5,5,5	0.46	0
2	GOL	B	601	-	5,5,5	0.39	0	5,5,5	0.96	0
3	EDO	B	602	-	3,3,3	0.86	0	2,2,2	1.42	0
3	EDO	C	605	-	3,3,3	1.09	0	2,2,2	1.02	0
2	GOL	C	607	-	5,5,5	0.55	0	5,5,5	0.75	0
2	GOL	D	600	-	5,5,5	0.19	0	5,5,5	0.41	0
5	TRS	C	603	-	7,7,7	0.57	0	9,9,9	2.30	4 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	C	601	-	3,3,3	0.88	0	2,2,2	0.90	0
3	EDO	A	602	-	3,3,3	0.34	0	2,2,2	0.54	0
3	EDO	C	609	-	3,3,3	1.64	1 (33%)	2,2,2	0.54	0
6	SIN	C	606	7	7,7,7	1.98	2 (28%)	8,8,8	1.04	0
2	GOL	C	608	-	5,5,5	0.85	0	5,5,5	1.83	2 (40%)
3	EDO	B	603	4	3,3,3	1.27	0	2,2,2	1.42	0
2	GOL	C	602	-	5,5,5	0.31	0	5,5,5	0.79	0
3	EDO	D	601	-	3,3,3	0.37	0	2,2,2	0.76	0
3	EDO	C	604	-	3,3,3	0.54	0	2,2,2	0.50	0
3	EDO	A	601	-	3,3,3	0.26	0	2,2,2	0.41	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
2	GOL	A	600	-	-	0/4/4/4	-
2	GOL	B	601	-	-	3/4/4/4	-
3	EDO	B	602	-	-	1/1/1/1	-
3	EDO	C	605	-	-	1/1/1/1	-
2	GOL	C	607	-	-	4/4/4/4	-
2	GOL	D	600	-	-	4/4/4/4	-
5	TRS	C	603	-	-	7/9/9/9	-
3	EDO	C	601	-	-	1/1/1/1	-
3	EDO	A	602	-	-	1/1/1/1	-
3	EDO	C	609	-	-	0/1/1/1	-
6	SIN	C	606	7	-	2/5/5/5	-
2	GOL	C	608	-	-	1/4/4/4	-
3	EDO	B	603	4	-	0/1/1/1	-
2	GOL	C	602	-	-	2/4/4/4	-
3	EDO	D	601	-	-	1/1/1/1	-
3	EDO	C	604	-	-	1/1/1/1	-
3	EDO	A	601	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	606	SIN	O4-C4	-3.95	1.17	1.30
6	C	606	SIN	O1-C1	2.42	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	609	EDO	O2-C2	2.40	1.54	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	603	TRS	C2-C-N	3.94	118.21	108.17
5	C	603	TRS	C2-C-C1	-3.62	101.03	110.66
5	C	603	TRS	O2-C2-C	-2.75	103.21	110.88
5	C	603	TRS	C3-C-C1	2.30	116.77	110.66
2	C	608	GOL	O3-C3-C2	2.15	120.05	110.38
2	C	608	GOL	C3-C2-C1	2.06	119.35	111.80

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	GOL	O1-C1-C2-O2
2	B	601	GOL	C1-C2-C3-O3
2	C	602	GOL	C1-C2-C3-O3
2	C	607	GOL	O1-C1-C2-O2
2	C	607	GOL	O1-C1-C2-C3
2	C	607	GOL	C1-C2-C3-O3
5	C	603	TRS	N-C-C3-O3
2	B	601	GOL	O1-C1-C2-C3
2	D	600	GOL	O1-C1-C2-C3
2	C	602	GOL	O2-C2-C3-O3
2	C	607	GOL	O2-C2-C3-O3
3	C	601	EDO	O1-C1-C2-O2
3	C	604	EDO	O1-C1-C2-O2
3	C	605	EDO	O1-C1-C2-O2
2	D	600	GOL	O1-C1-C2-O2
5	C	603	TRS	N-C-C2-O2
2	D	600	GOL	C1-C2-C3-O3
5	C	603	TRS	N-C-C1-O1
5	C	603	TRS	C1-C-C2-O2
6	C	606	SIN	O1-C1-C2-C3
2	C	608	GOL	O1-C1-C2-O2
2	D	600	GOL	O2-C2-C3-O3
3	D	601	EDO	O1-C1-C2-O2
6	C	606	SIN	O2-C1-C2-C3
5	C	603	TRS	C3-C-C1-O1
5	C	603	TRS	C1-C-C3-O3

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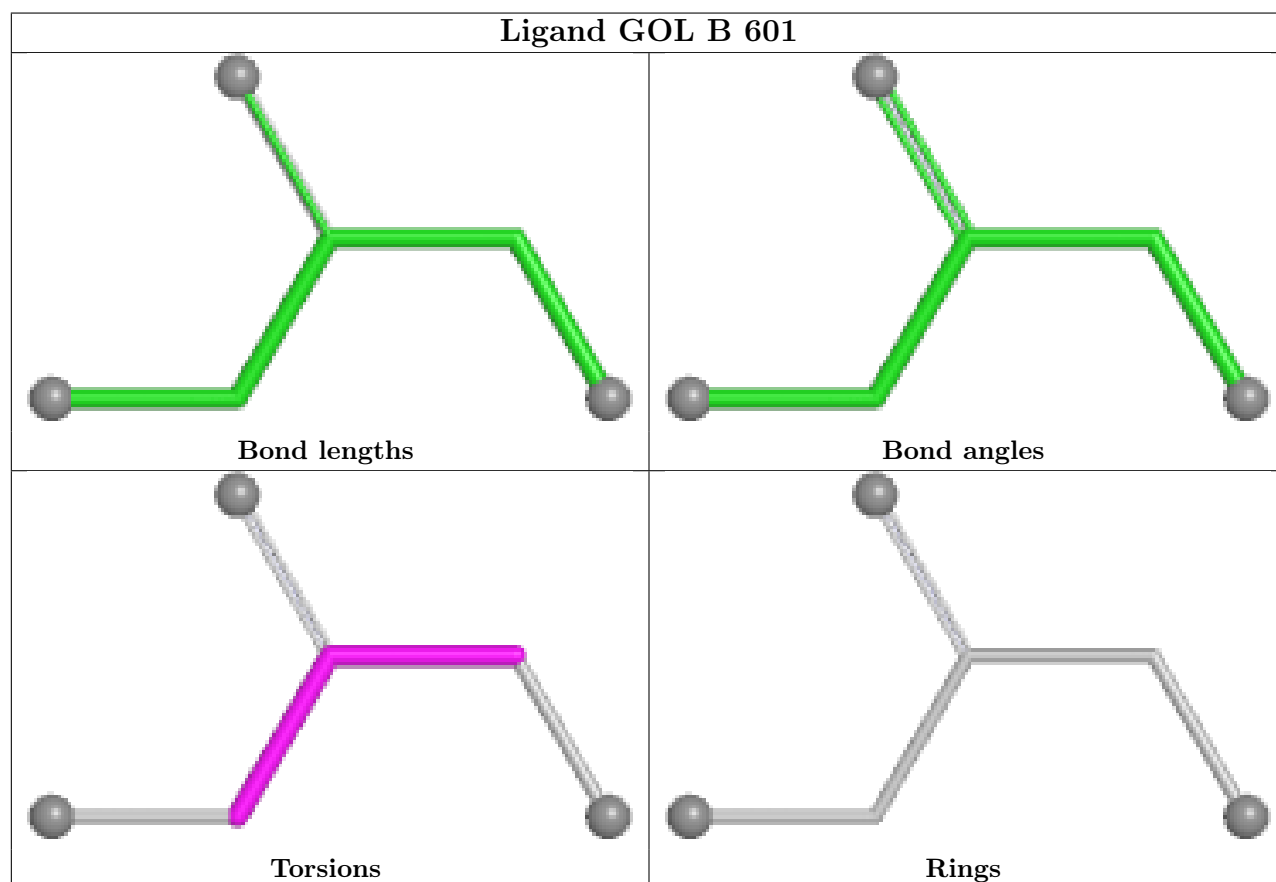
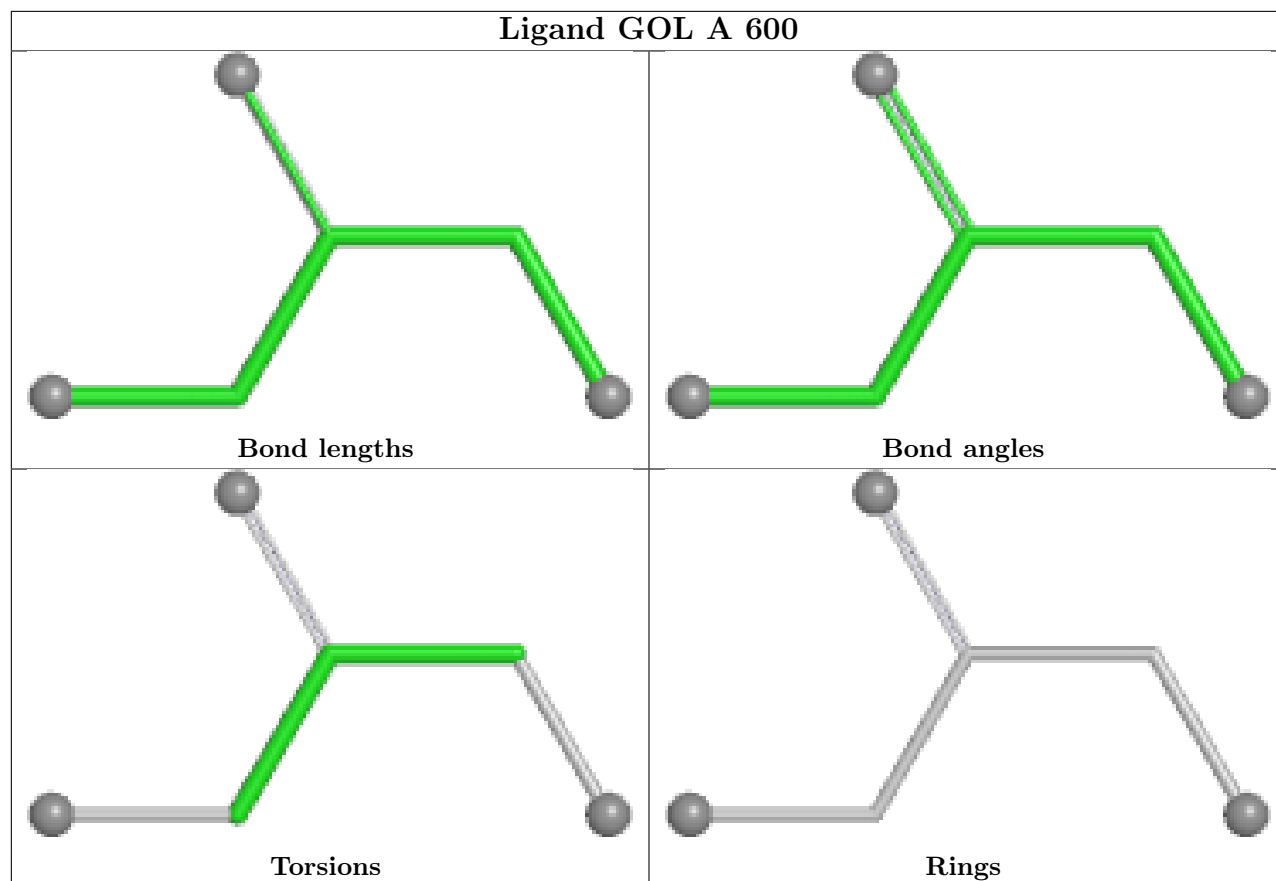
Mol	Chain	Res	Type	Atoms
5	C	603	TRS	C2-C-C3-O3
3	A	602	EDO	O1-C1-C2-O2
3	B	602	EDO	O1-C1-C2-O2

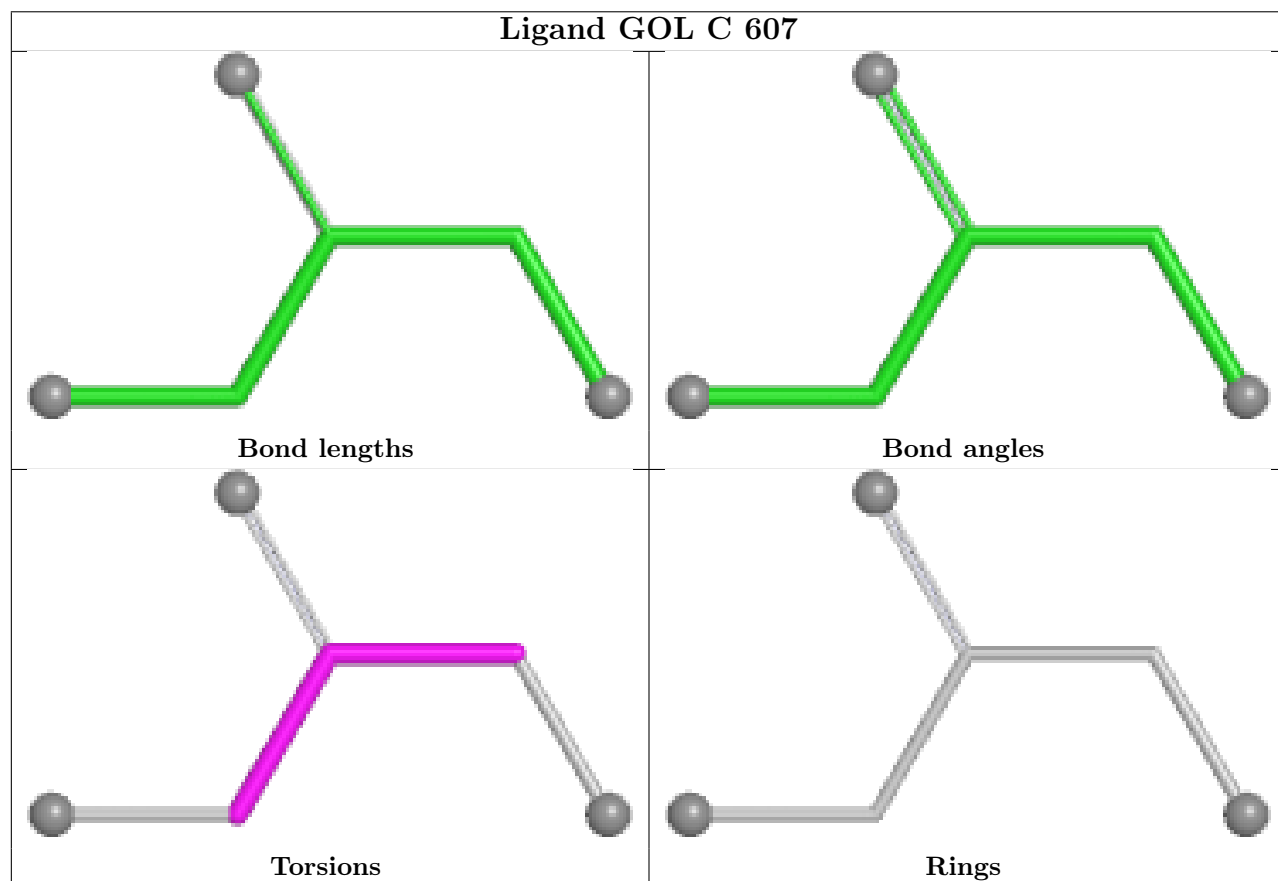
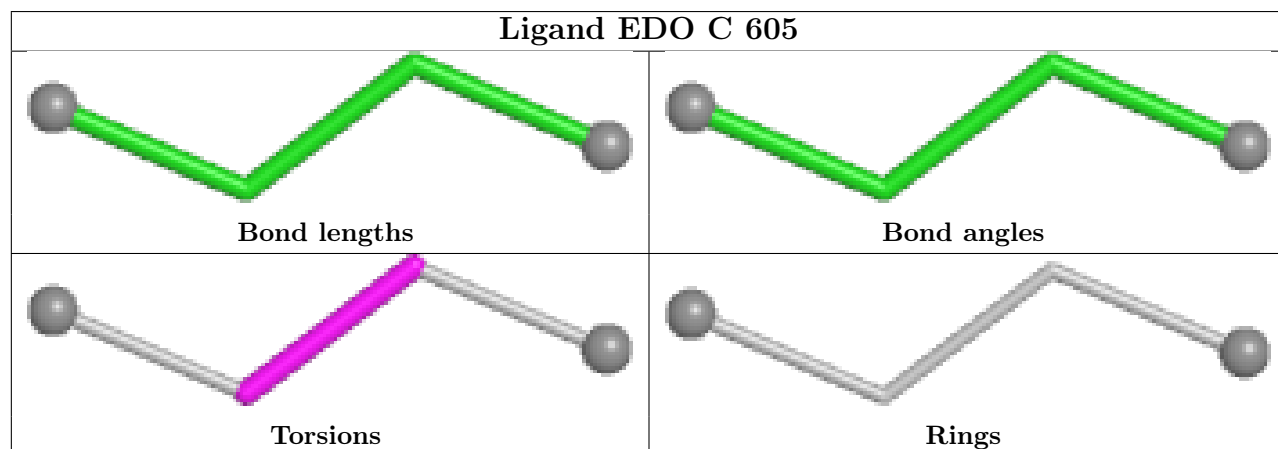
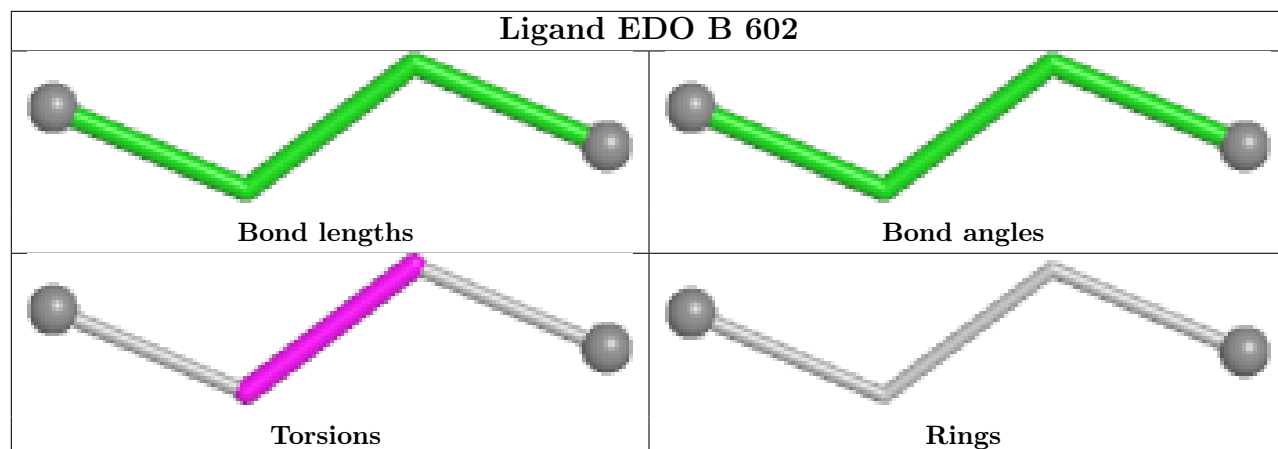
There are no ring outliers.

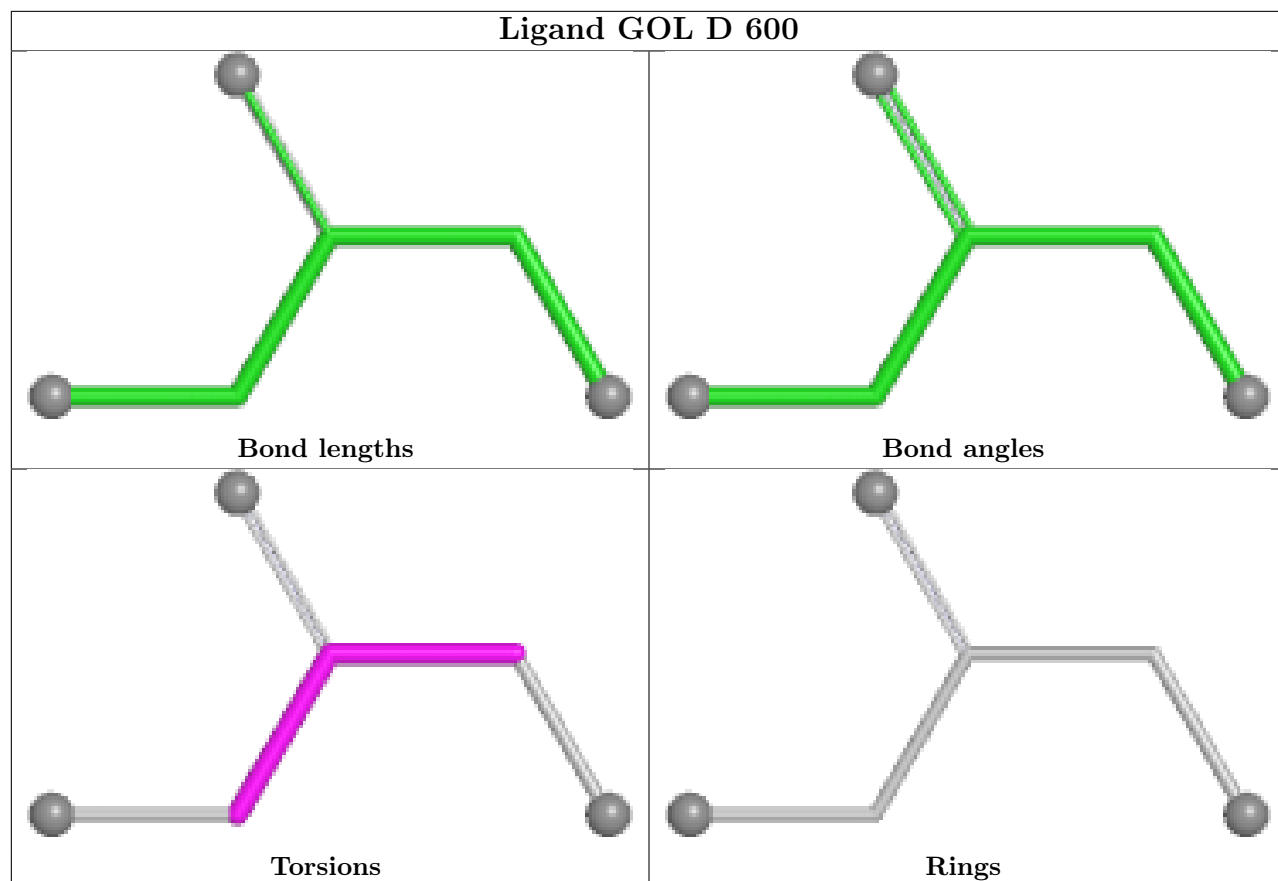
6 monomers are involved in 8 short contacts:

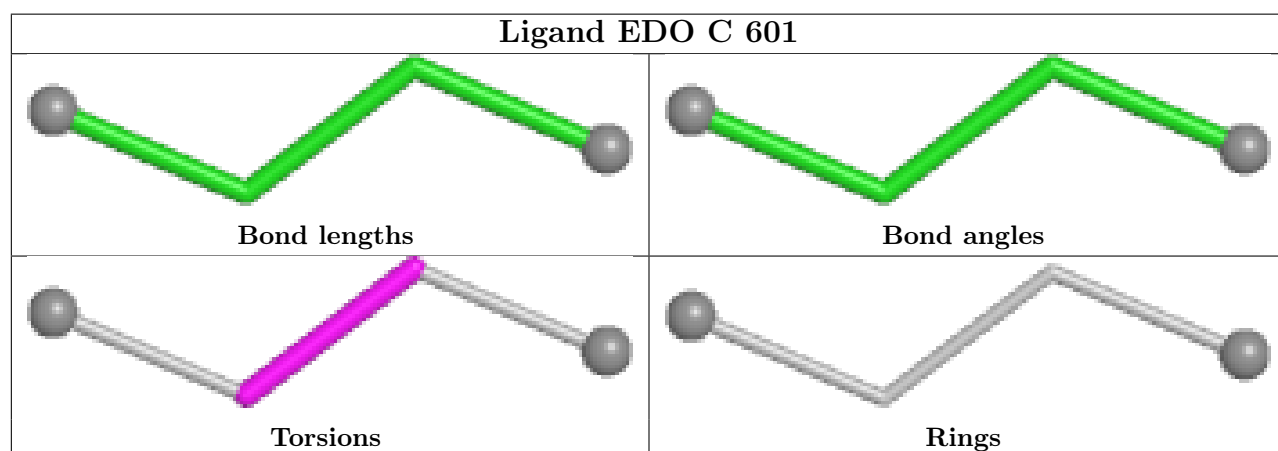
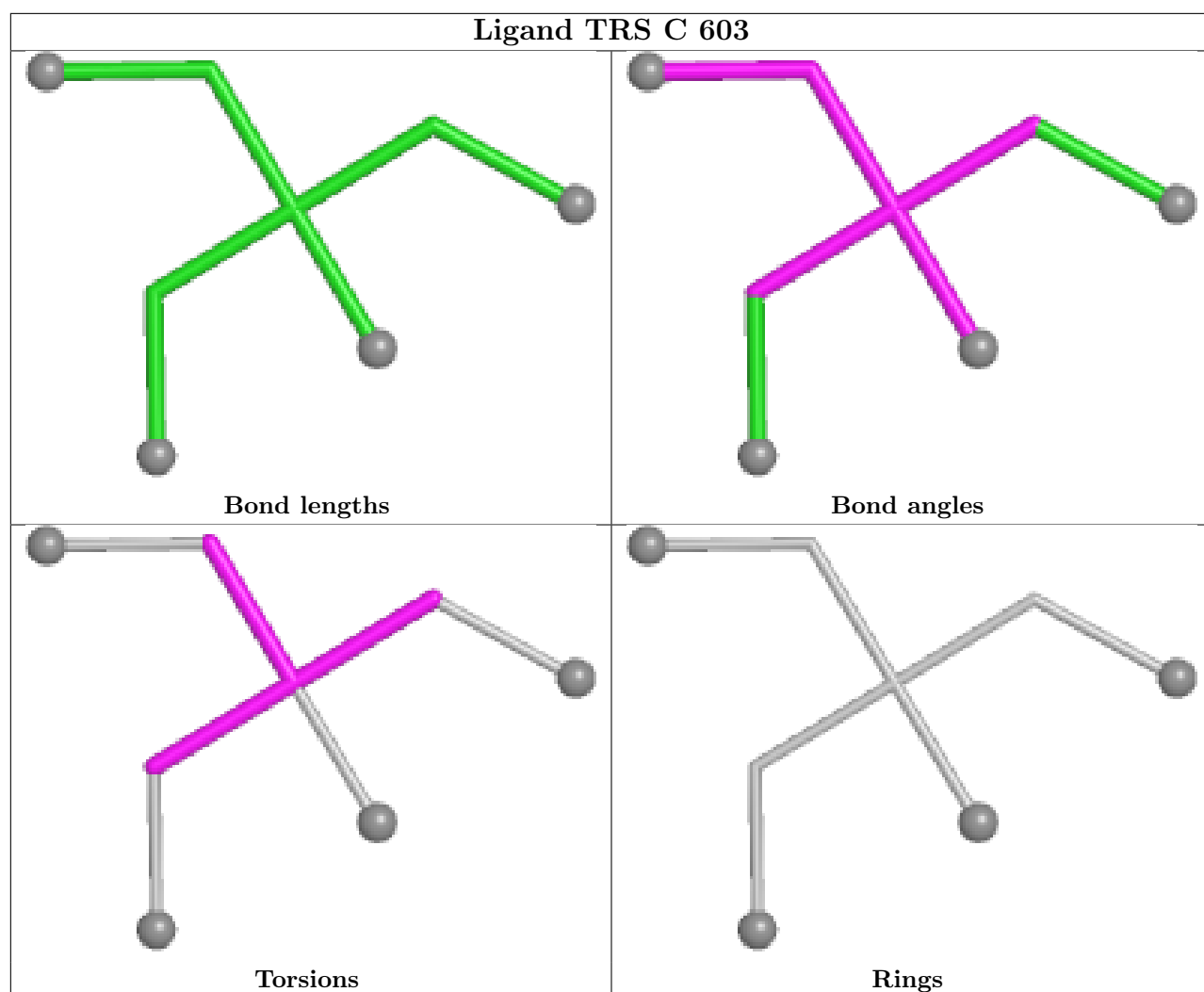
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	GOL	1	0
2	C	607	GOL	1	0
5	C	603	TRS	3	0
3	C	609	EDO	2	0
6	C	606	SIN	1	0
2	C	608	GOL	3	0

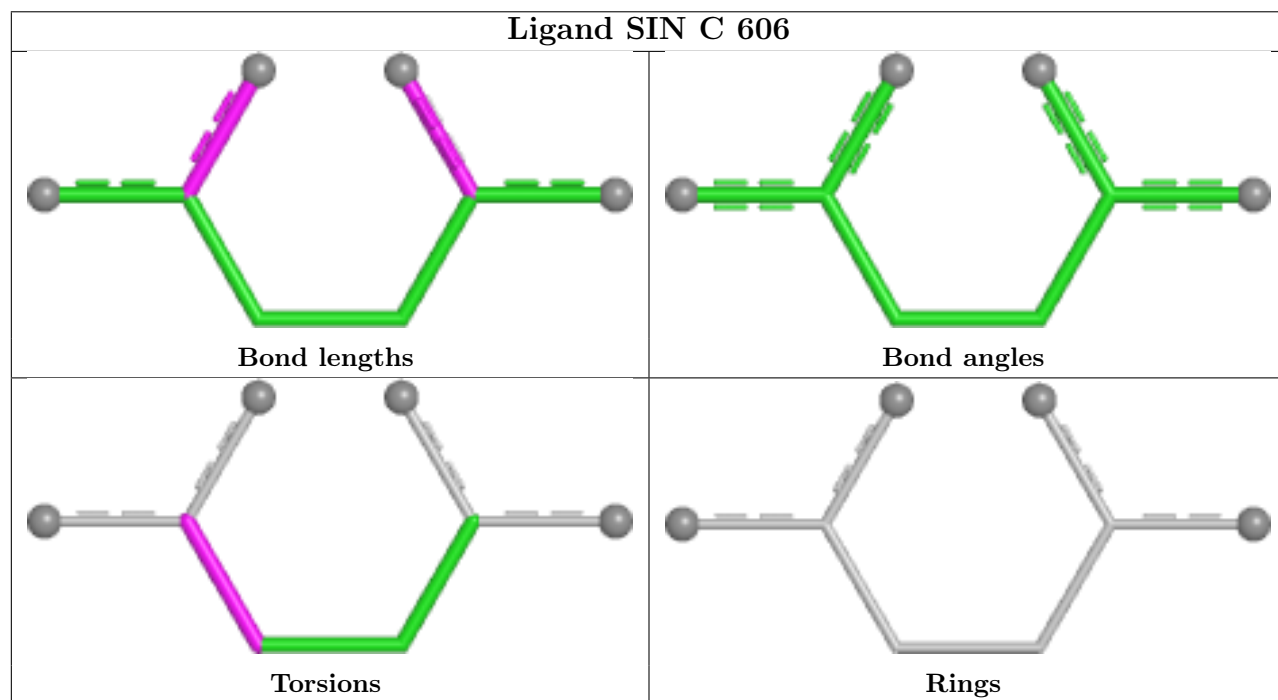
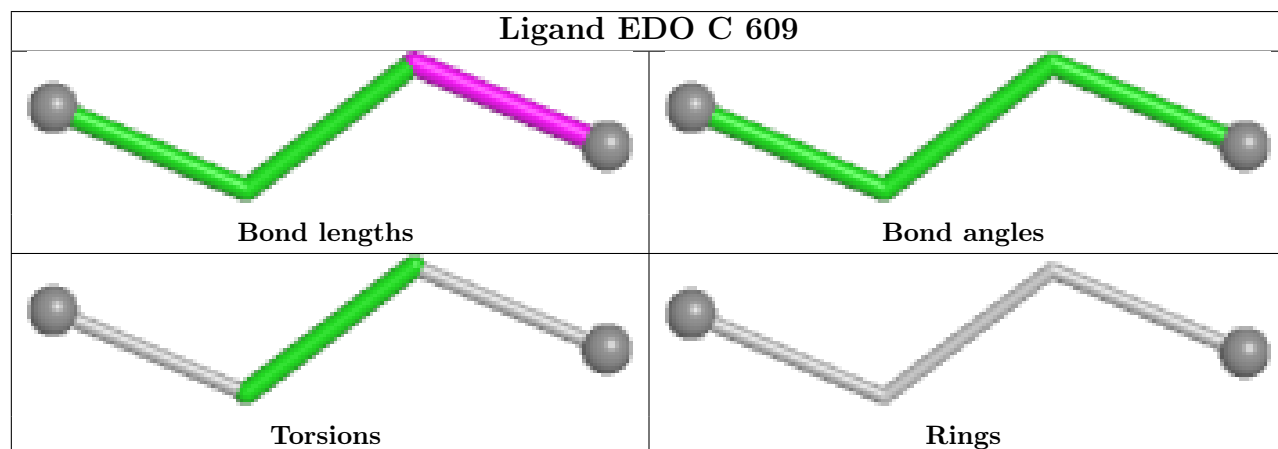
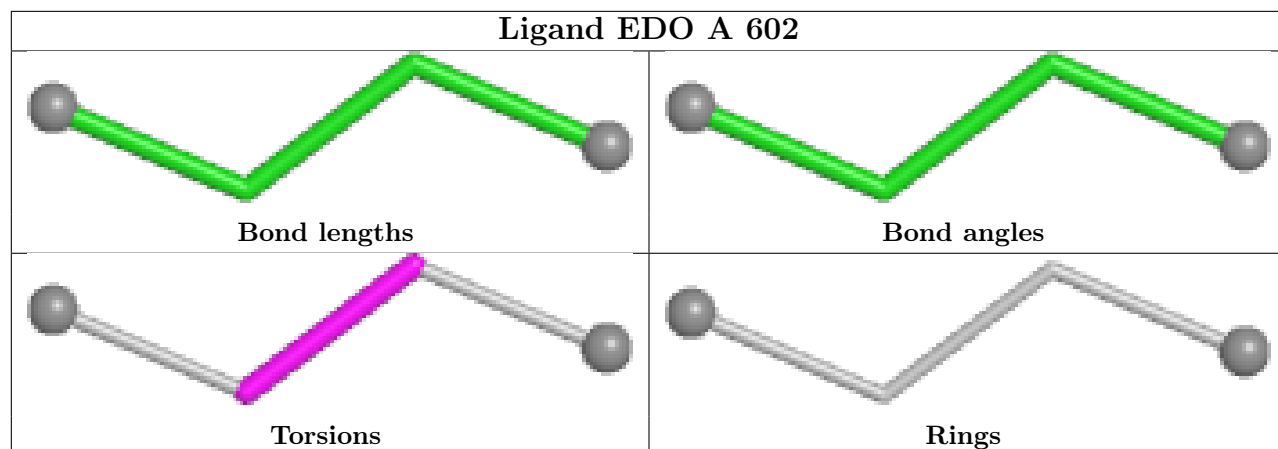
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

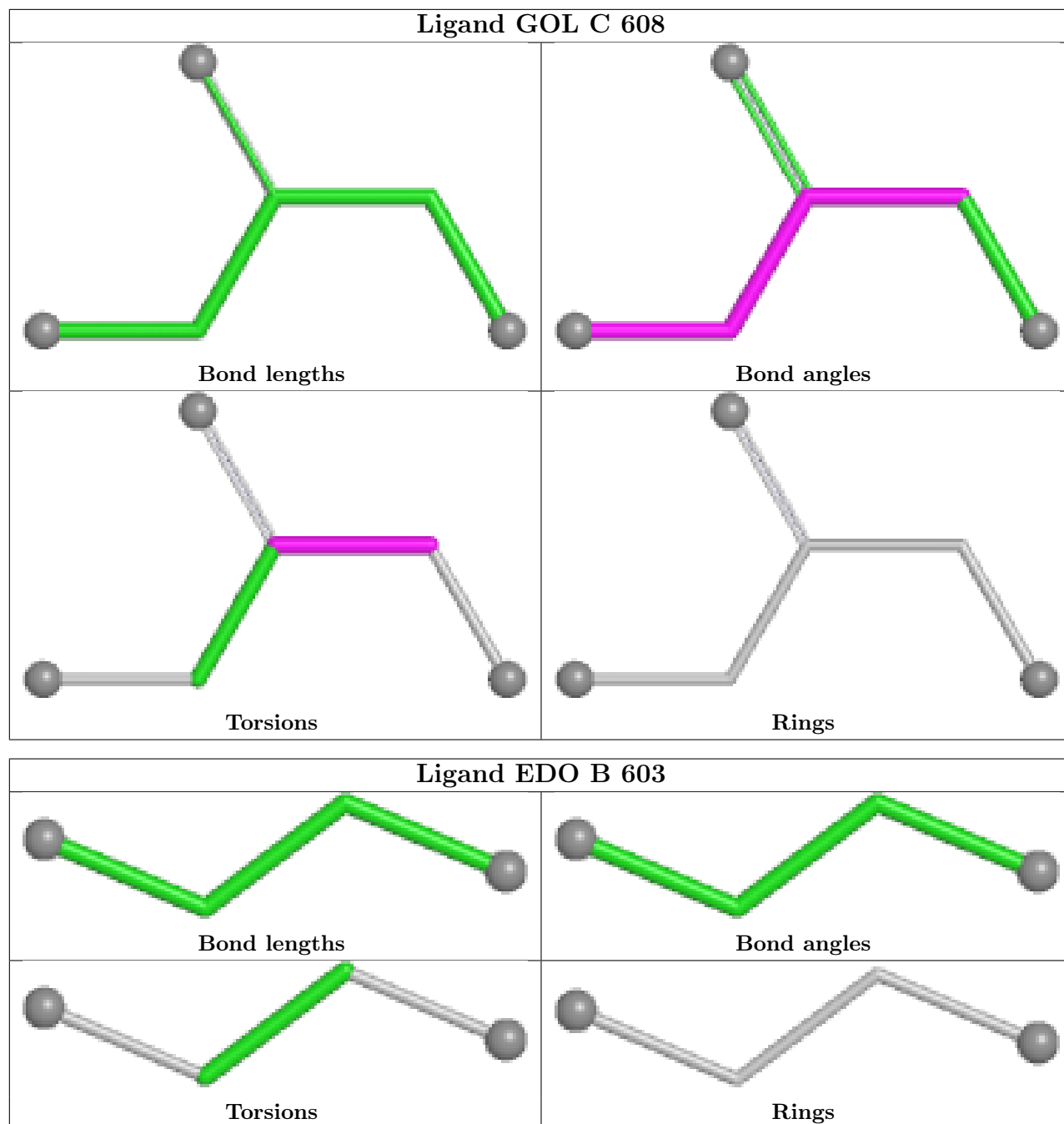


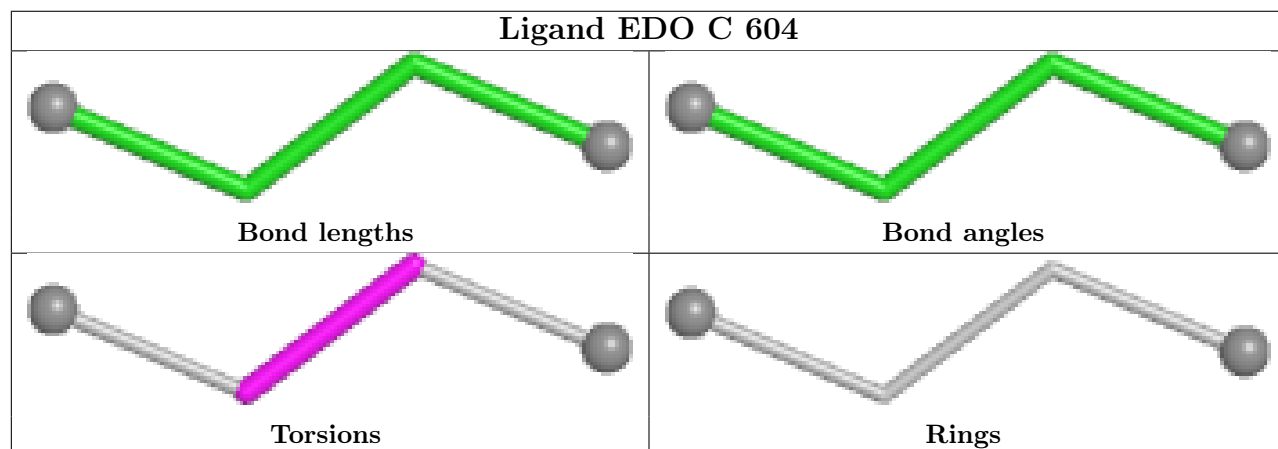
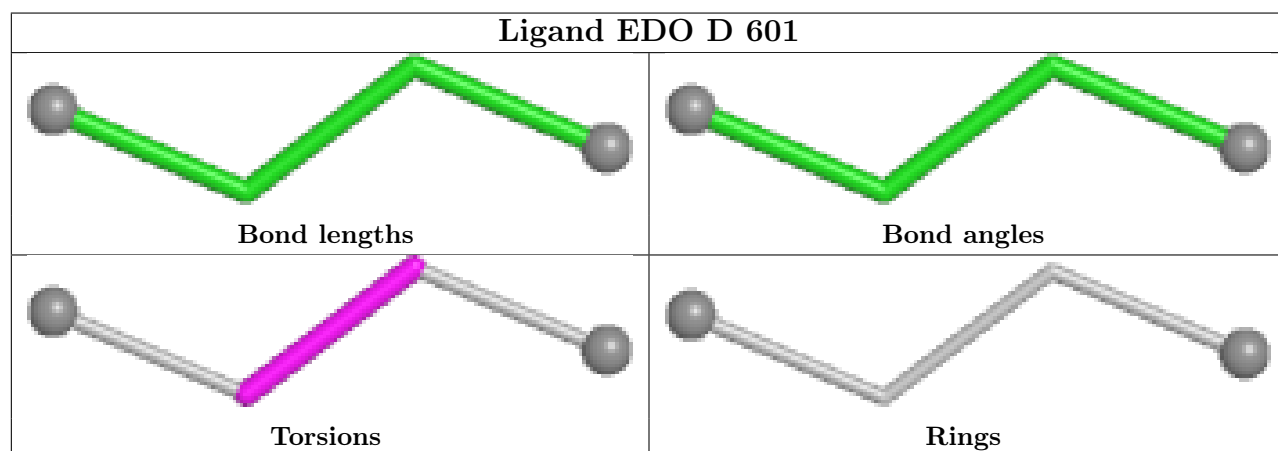
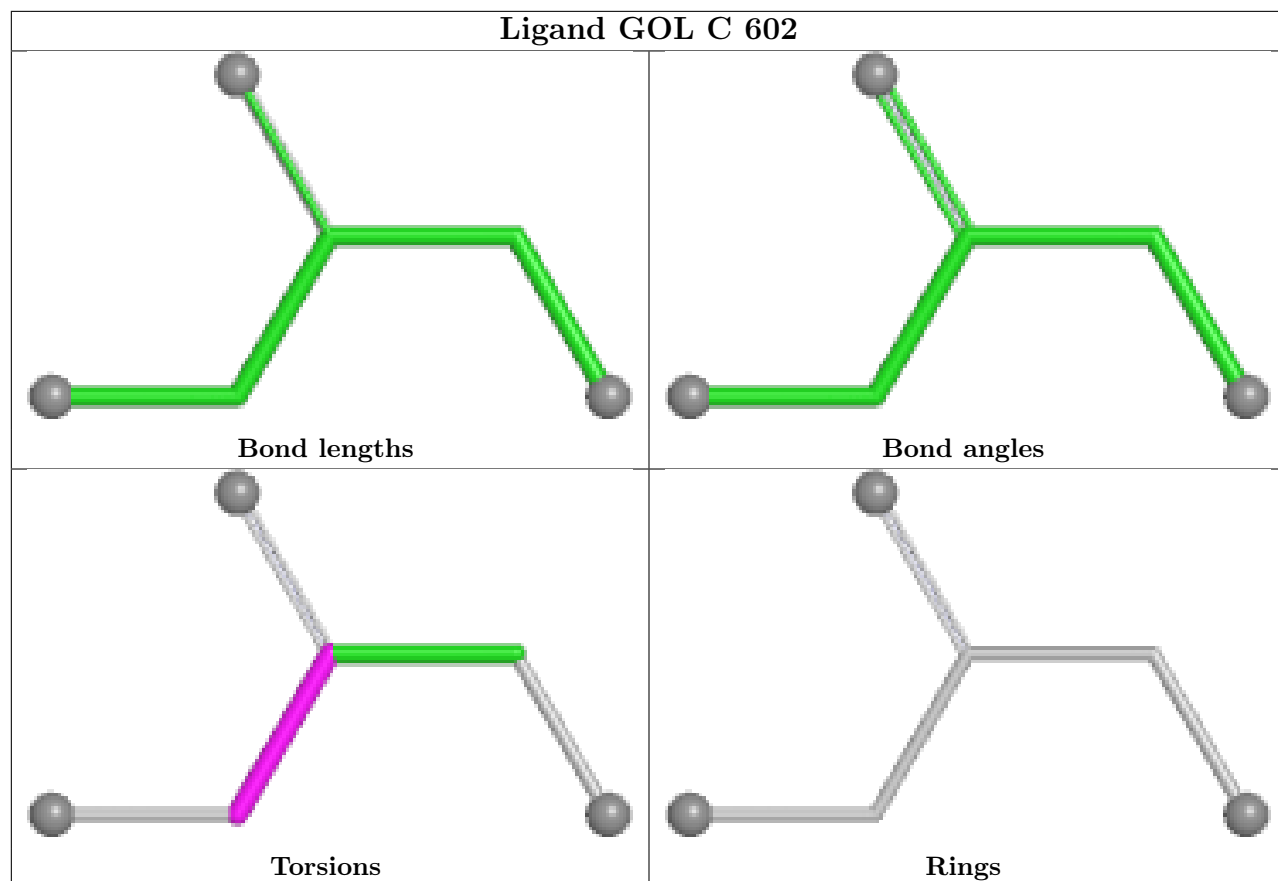


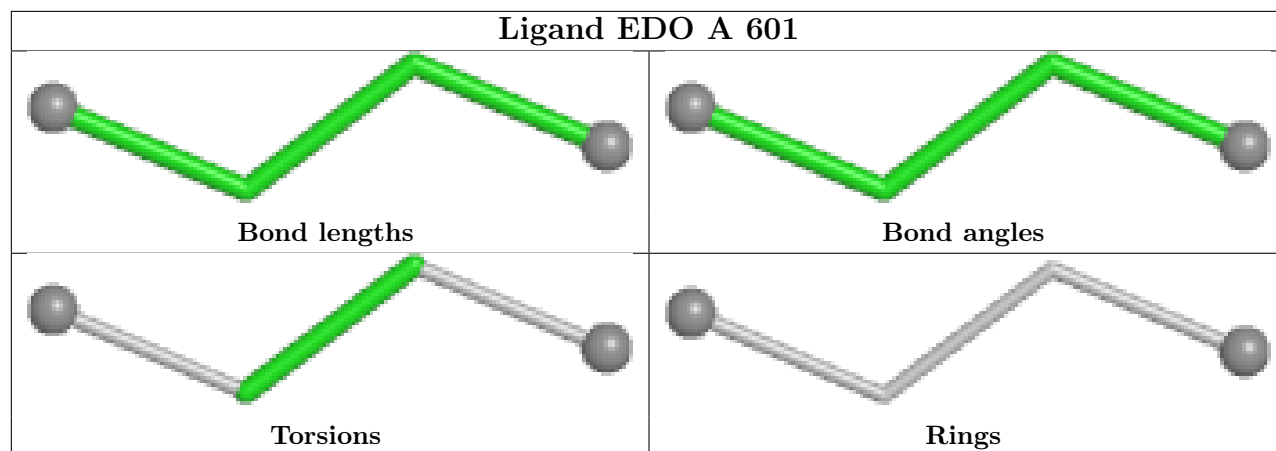












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	504/537 (93%)	0.86	55 (10%)	10 9	24, 67, 117, 150	2 (0%)
1	B	516/537 (96%)	0.42	41 (7%)	18 18	31, 50, 104, 120	0
1	C	512/537 (95%)	0.30	29 (5%)	29 28	24, 52, 89, 113	1 (0%)
1	D	501/537 (93%)	1.59	157 (31%)	1 1	49, 87, 159, 185	0
All	All	2033/2148 (94%)	0.79	282 (13%)	6 5	24, 63, 120, 185	3 (0%)

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	ILE	8.4
1	D	159	LEU	6.5
1	D	117	PRO	6.4
1	A	326	CYS	6.1
1	D	134	LEU	5.6
1	D	237	VAL	5.3
1	D	519	SER	5.3
1	B	128	GLY	5.1
1	D	157	LEU	5.1
1	D	209	VAL	4.9
1	D	170	VAL	4.9
1	D	156	ILE	4.5
1	A	358	CYS	4.5
1	C	404	ILE	4.4
1	A	521	PHE	4.4
1	D	158	TRP	4.4
1	D	404	ILE	4.2
1	D	138	ALA	4.1
1	A	190	ALA	4.0
1	C	158	TRP	4.0
1	A	152	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	192	PHE	3.9
1	D	470	PHE	3.9
1	D	482	TRP	3.9
1	B	520	GLY	3.8
1	C	130	ALA	3.8
1	B	517	PRO	3.8
1	D	40	ILE	3.8
1	D	520	GLY	3.7
1	D	203	LEU	3.6
1	A	137	GLY	3.6
1	B	170	VAL	3.6
1	A	341	THR	3.6
1	D	144	LEU	3.6
1	D	403	PRO	3.6
1	C	148	TYR	3.6
1	A	121	THR	3.6
1	A	533	HIS	3.6
1	C	159	LEU	3.5
1	C	403	PRO	3.5
1	D	488	LEU	3.5
1	D	421	PHE	3.4
1	D	431	LEU	3.4
1	B	533	HIS	3.4
1	D	292	VAL	3.4
1	C	40	ILE	3.4
1	D	518	GLY	3.4
1	A	192	PHE	3.4
1	D	141	LYS	3.4
1	B	532	HIS	3.4
1	D	521	PHE	3.3
1	C	136	LYS	3.3
1	B	190	ALA	3.3
1	D	190	ALA	3.3
1	D	517	PRO	3.2
1	B	404	ILE	3.2
1	C	470	PHE	3.2
1	D	143	THR	3.2
1	D	216	VAL	3.2
1	D	293	ALA	3.2
1	D	254	VAL	3.1
1	D	140	LEU	3.1
1	A	470	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	327	ALA	3.1
1	C	401	LEU	3.1
1	D	361	LEU	3.1
1	D	148	TYR	3.1
1	D	50	THR	3.1
1	B	430	VAL	3.1
1	D	65	ILE	3.1
1	A	515	TRP	3.1
1	D	274	HIS	3.1
1	C	119	ILE	3.1
1	A	149	MET	3.0
1	D	204	GLY	3.0
1	D	188	LYS	3.0
1	D	512	LEU	3.0
1	A	335	ILE	3.0
1	A	518	GLY	3.0
1	A	139	THR	3.0
1	D	522	THR	3.0
1	D	58	VAL	3.0
1	D	171	GLY	2.9
1	A	151	LYS	2.9
1	D	76	PHE	2.9
1	D	175	TYR	2.9
1	D	515	TRP	2.9
1	D	147	ALA	2.9
1	A	180	LEU	2.9
1	A	203	LEU	2.9
1	D	74	LEU	2.9
1	D	60	THR	2.9
1	D	102	PRO	2.9
1	D	83	TYR	2.9
1	A	353	LEU	2.9
1	D	194	VAL	2.9
1	A	50	THR	2.9
1	A	138	ALA	2.9
1	D	116	GLY	2.9
1	D	453	VAL	2.8
1	A	142	ILE	2.8
1	B	518	GLY	2.8
1	B	203	LEU	2.8
1	B	129	THR	2.8
1	A	482	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	40	ILE	2.8
1	B	147	ALA	2.8
1	D	112	LEU	2.8
1	D	504	LYS	2.8
1	D	165	CYS	2.8
1	B	436	ARG	2.7
1	A	363	GLY	2.7
1	D	48	ILE	2.7
1	A	532	HIS	2.7
1	B	521	PHE	2.7
1	C	532	HIS	2.7
1	B	400	ARG	2.7
1	B	470	PHE	2.7
1	D	180	LEU	2.7
1	D	164	ILE	2.7
1	D	174	ILE	2.7
1	D	417	VAL	2.7
1	D	152	CYS	2.7
1	B	515	TRP	2.7
1	D	215	ALA	2.6
1	D	452	ALA	2.6
1	D	444	TYR	2.6
1	C	135	LYS	2.6
1	D	433	LYS	2.6
1	D	436	ARG	2.6
1	C	144	LEU	2.6
1	D	503	PHE	2.6
1	D	481	ALA	2.6
1	B	157	LEU	2.6
1	D	505	LYS	2.6
1	B	14	GLN	2.6
1	D	168	VAL	2.6
1	D	271	ILE	2.6
1	C	505	LYS	2.6
1	A	522	THR	2.6
1	D	401	LEU	2.6
1	D	465	LEU	2.6
1	D	299	ILE	2.5
1	D	472	VAL	2.5
1	B	189	GLY	2.5
1	D	506	GLY	2.5
1	A	148	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	440	GLN	2.5
1	A	157	LEU	2.5
1	A	189	GLY	2.5
1	A	156	ILE	2.5
1	C	15	THR	2.5
1	D	331	LEU	2.5
1	D	22	MET	2.5
1	D	66	LYS	2.5
1	D	98	PHE	2.5
1	A	345	GLY	2.5
1	D	428	ILE	2.5
1	A	437	SER	2.4
1	D	420	SER	2.4
1	D	99	ALA	2.4
1	B	123	LEU	2.4
1	B	192	PHE	2.4
1	D	244	PHE	2.4
1	D	221	VAL	2.4
1	D	301	ILE	2.4
1	D	405	THR	2.4
1	D	302	PRO	2.4
1	D	531	PRO	2.4
1	D	443	ARG	2.4
1	A	183	LEU	2.4
1	D	232	GLY	2.4
1	C	192	PHE	2.4
1	C	24	ASP	2.4
1	D	51	ILE	2.4
1	D	226	ILE	2.4
1	D	277	VAL	2.4
1	A	370	TYR	2.4
1	D	435	GLY	2.4
1	A	436	ARG	2.4
1	C	194	VAL	2.4
1	D	265	ILE	2.4
1	D	45	THR	2.4
1	A	517	PRO	2.4
1	D	457	PRO	2.4
1	D	218	LEU	2.3
1	D	473	LEU	2.3
1	D	231	PHE	2.3
1	B	159	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	502	PHE	2.3
1	D	267	ILE	2.3
1	A	340	PRO	2.3
1	D	114	THR	2.3
1	D	524	THR	2.3
1	D	343	ALA	2.3
1	B	134	LEU	2.3
1	B	180	LEU	2.3
1	B	201	GLY	2.3
1	B	482	TRP	2.3
1	A	181	ILE	2.3
1	C	156	ILE	2.3
1	D	181	ILE	2.3
1	B	139	THR	2.3
1	D	219	PRO	2.3
1	A	226	ILE	2.2
1	D	93	THR	2.2
1	D	185	VAL	2.2
1	D	530	VAL	2.2
1	A	399	ARG	2.2
1	D	500	ARG	2.2
1	B	130	ALA	2.2
1	D	64	MET	2.2
1	D	111	ALA	2.2
1	D	189	GLY	2.2
1	D	201	GLY	2.2
1	D	213	GLY	2.2
1	D	214	ALA	2.2
1	A	78	HIS	2.2
1	A	158	TRP	2.2
1	A	227	GLN	2.2
1	A	519	SER	2.2
1	B	132	VAL	2.2
1	C	22	MET	2.2
1	A	206	LYS	2.2
1	B	505	LYS	2.2
1	D	146	ASN	2.2
1	D	325	ILE	2.2
1	D	91	VAL	2.2
1	A	204	GLY	2.2
1	C	123	LEU	2.2
1	D	372	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	202	SER	2.2
1	C	400	ARG	2.2
1	D	106	ARG	2.2
1	D	135	LYS	2.2
1	D	206	LYS	2.2
1	B	405	THR	2.2
1	D	110	VAL	2.1
1	D	440	GLN	2.1
1	C	405	THR	2.1
1	D	245	ILE	2.1
1	A	176	VAL	2.1
1	B	204	GLY	2.1
1	D	252	HIS	2.1
1	D	486	VAL	2.1
1	D	447	ARG	2.1
1	D	303	ALA	2.1
1	C	134	LEU	2.1
1	D	104	LEU	2.1
1	D	507	ASP	2.1
1	A	175	TYR	2.1
1	A	520	GLY	2.1
1	B	179	GLY	2.1
1	D	335	ILE	2.1
1	D	478	VAL	2.1
1	D	166	LYS	2.1
1	D	402	ALA	2.1
1	D	177	ASP	2.1
1	D	191	ASP	2.1
1	B	148	TYR	2.1
1	C	370	TYR	2.1
1	D	87	THR	2.1
1	C	164	ILE	2.1
1	D	240	VAL	2.1
1	D	508	VAL	2.1
1	D	149	MET	2.0
1	B	522	THR	2.0
1	A	173	LYS	2.0
1	A	68	GLY	2.0
1	A	103	ILE	2.0
1	D	395	PHE	2.0
1	B	463	ALA	2.0
1	C	190	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	382	ALA	2.0
1	C	14	GLN	2.0
1	D	14	GLN	2.0
1	D	73	ARG	2.0
1	D	151	LYS	2.0
1	B	524	THR	2.0
1	D	80	THR	2.0
1	D	477	PRO	2.0
1	D	179	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	ALY	D	115	12/13	0.63	0.21	105,114,121,122	0
1	ALY	A	115	12/13	0.69	0.19	69,77,90,92	0
1	ALY	C	115	12/13	0.86	0.14	50,59,81,88	0
1	ALY	B	115	12/13	0.88	0.15	45,56,80,90	0

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
2	GOL	C	607	6/6	0.67	0.22	70,84,88,92	0
3	EDO	A	601	4/4	0.73	0.19	88,91,92,93	0
3	EDO	D	601	4/4	0.76	0.22	80,82,84,87	0
3	EDO	A	602	4/4	0.80	0.14	60,61,62,64	0
2	GOL	C	608	6/6	0.80	0.20	42,43,44,44	0

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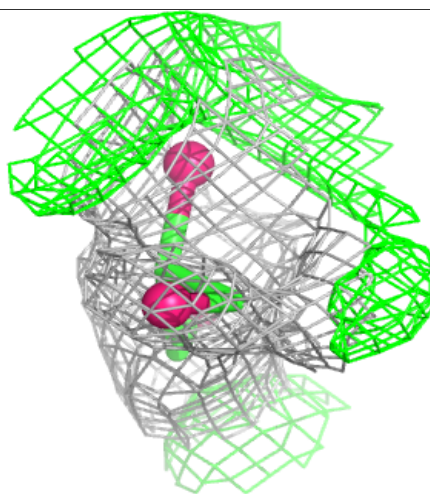
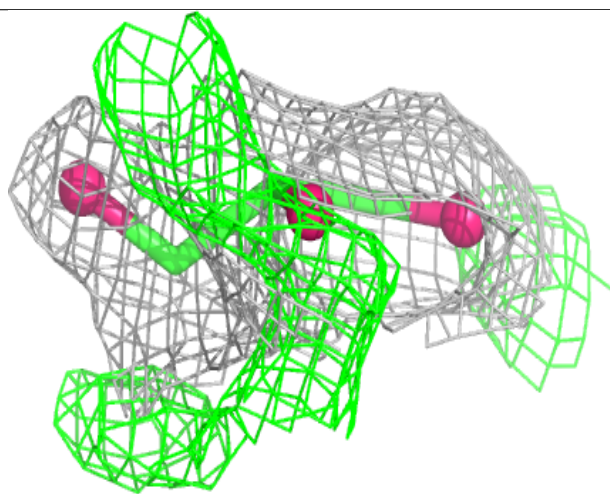
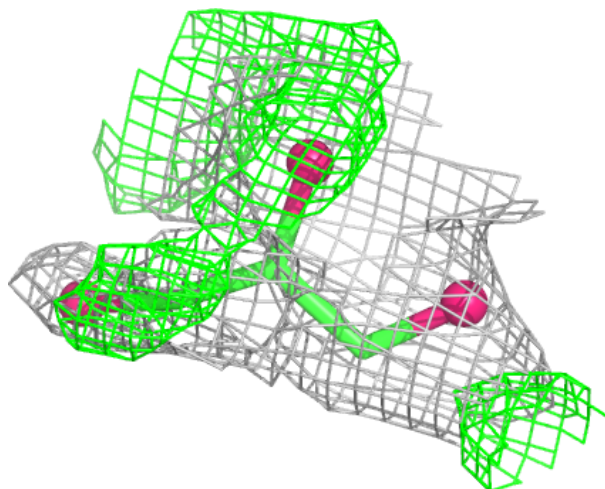
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	C	609	4/4	0.82	0.25	46,47,47,48	0
2	GOL	B	601	6/6	0.83	0.17	53,62,63,67	0
3	EDO	C	605	4/4	0.84	0.22	64,68,70,71	0
5	TRS	C	603	8/8	0.86	0.17	52,54,55,60	0
3	EDO	C	601	4/4	0.87	0.17	54,55,55,61	0
2	GOL	A	600	6/6	0.88	0.13	64,71,72,73	0
7	K	C	610	1/1	0.88	0.16	72,72,72,72	0
6	SIN	C	606	8/8	0.89	0.11	48,59,72,74	0
2	GOL	D	600	6/6	0.89	0.11	80,82,84,85	0
3	EDO	B	603	4/4	0.90	0.12	43,45,47,49	0
3	EDO	B	602	4/4	0.90	0.17	52,54,54,55	0
2	GOL	C	602	6/6	0.91	0.13	57,60,65,66	0
4	MG	B	604	1/1	0.94	0.06	51,51,51,51	0
3	EDO	C	604	4/4	0.94	0.11	58,59,59,60	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.

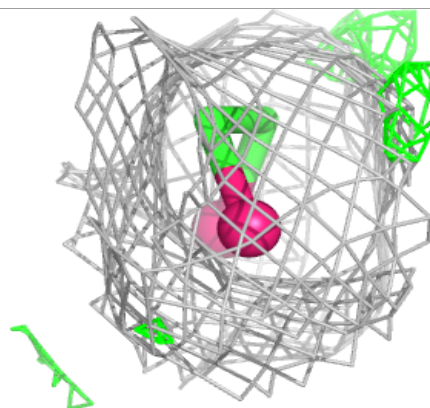
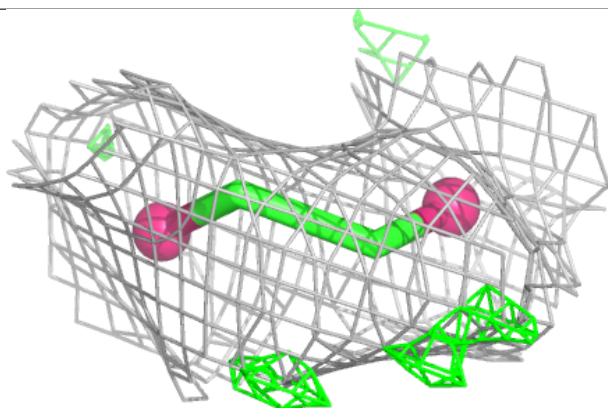
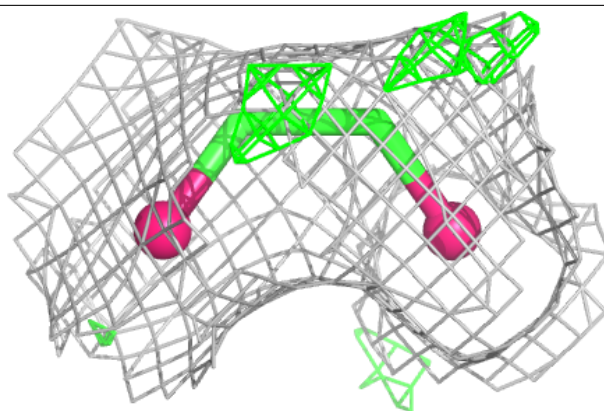
Electron density around GOL C 607:

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

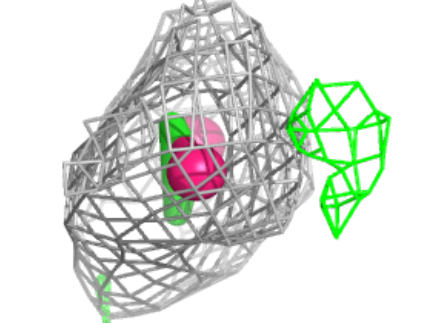
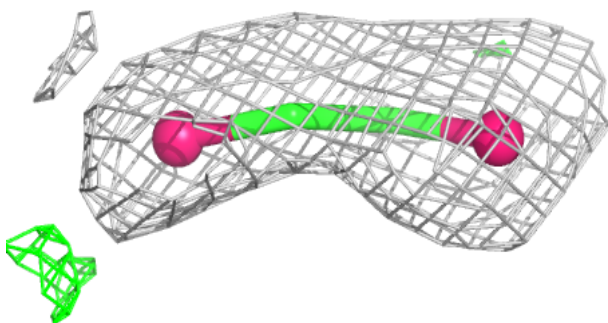
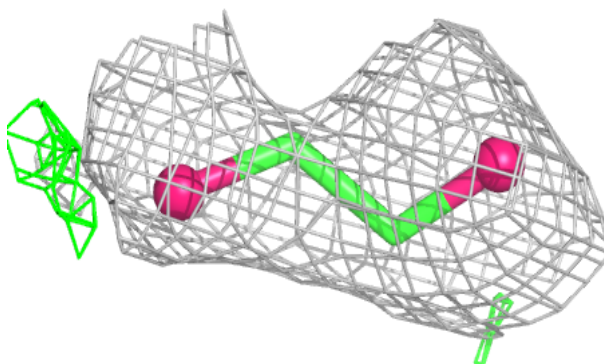


Electron density around EDO A 601:

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

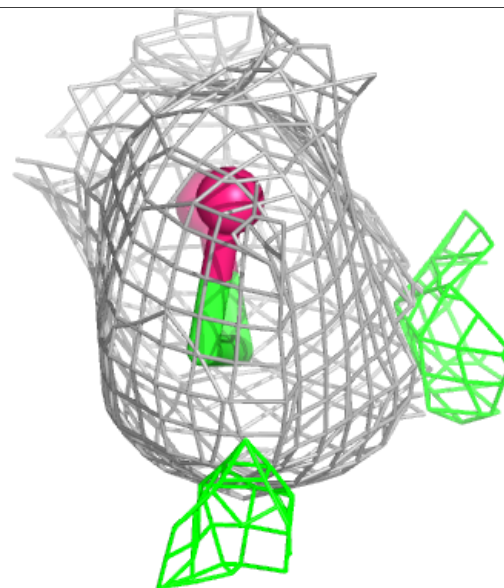
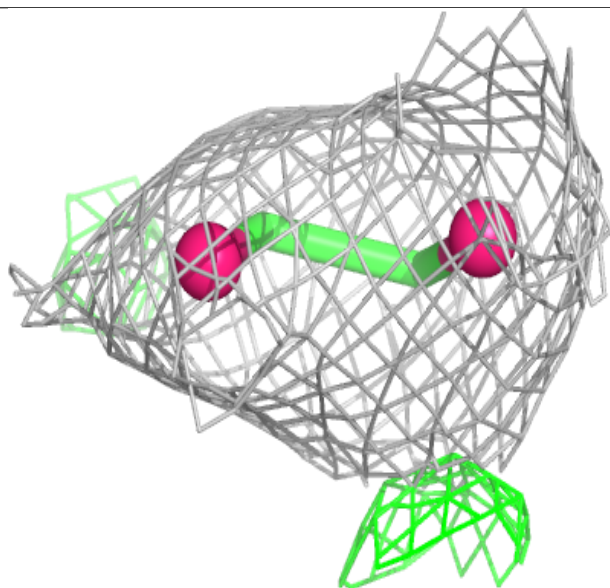
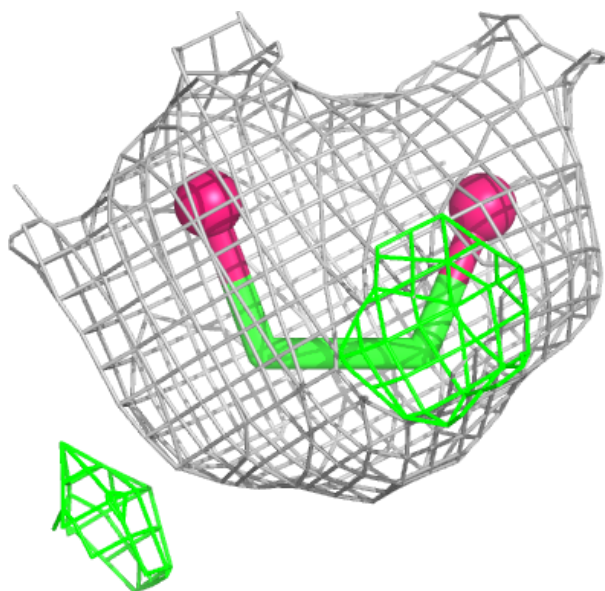
**Electron density around EDO D 601:**

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



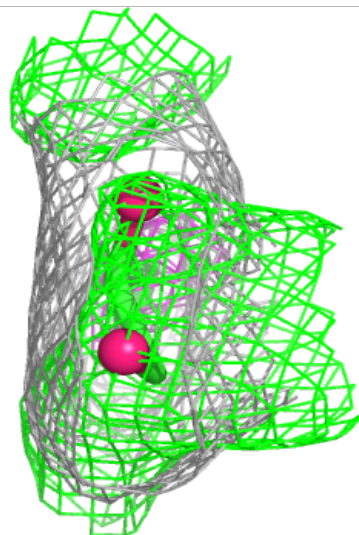
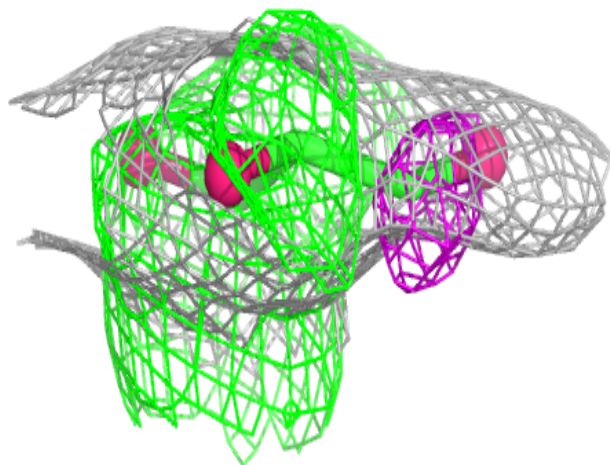
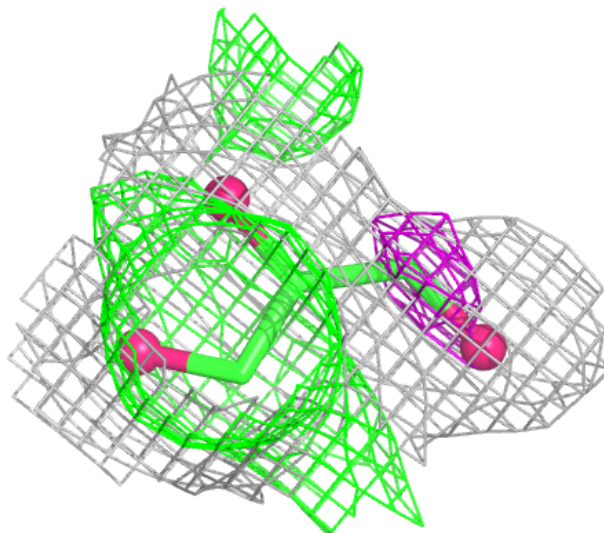
Electron density around EDO A 602:

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



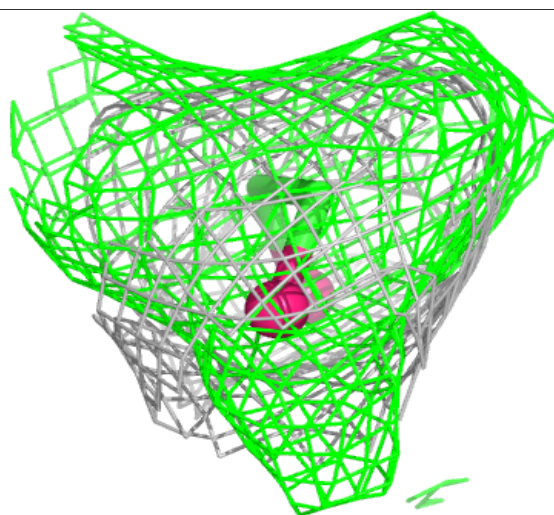
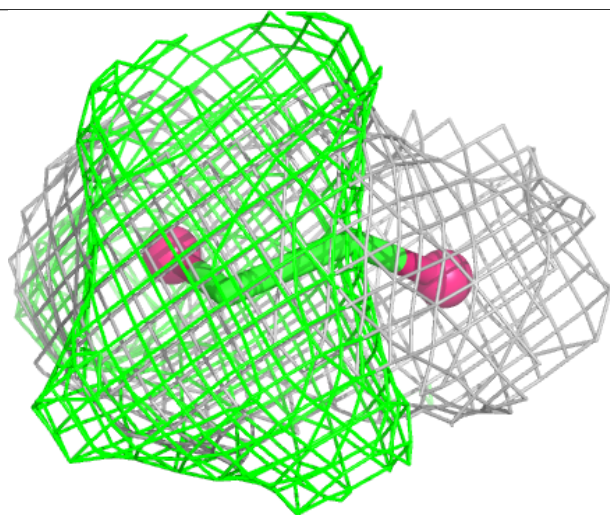
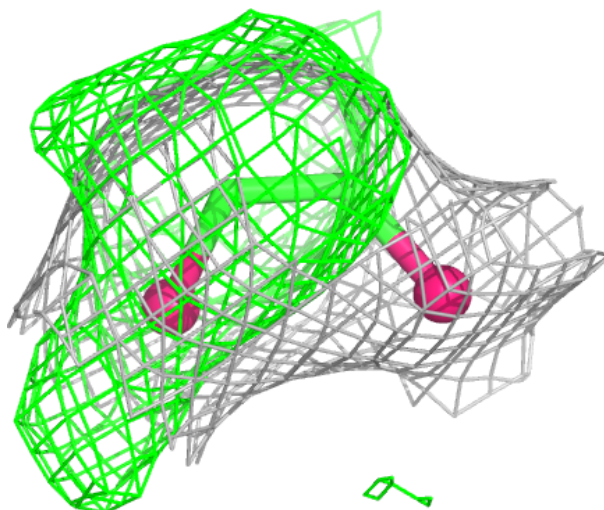
Electron density around GOL C 608:

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



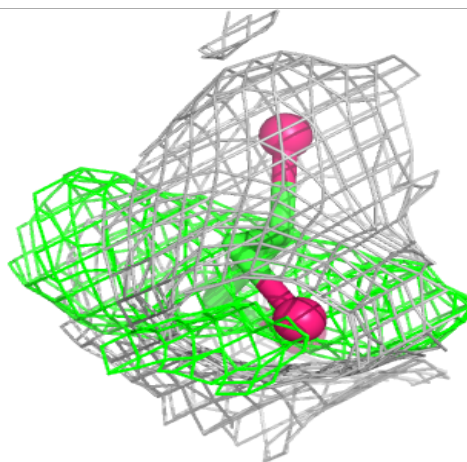
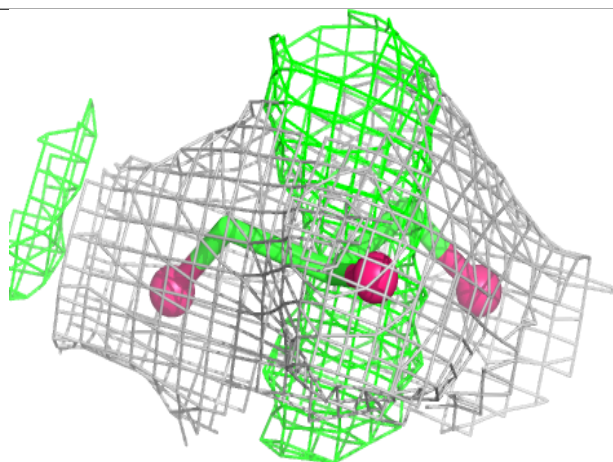
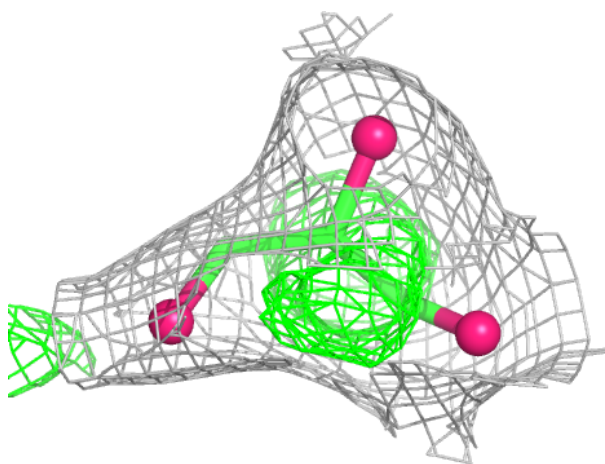
Electron density around EDO C 609:

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



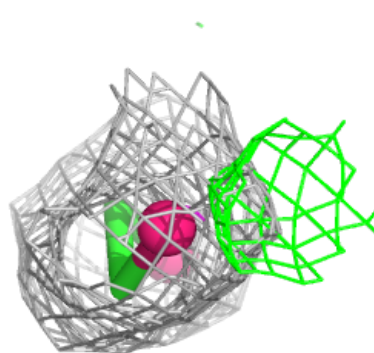
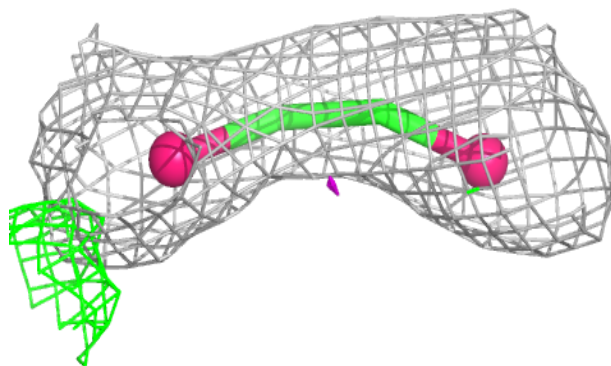
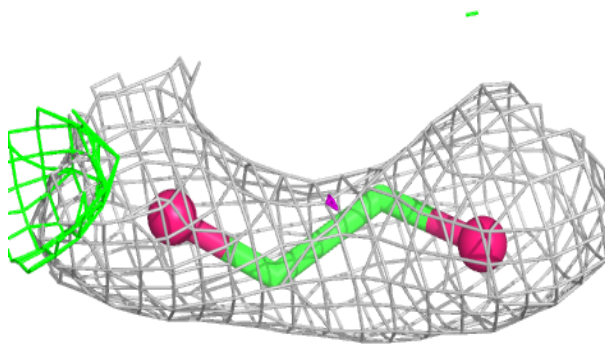
Electron density around GOL B 601:

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



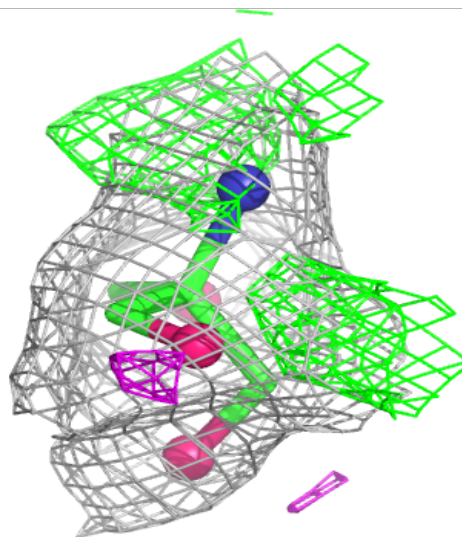
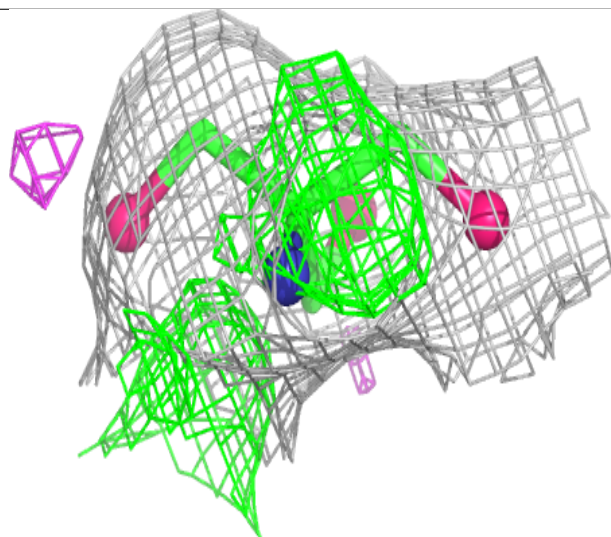
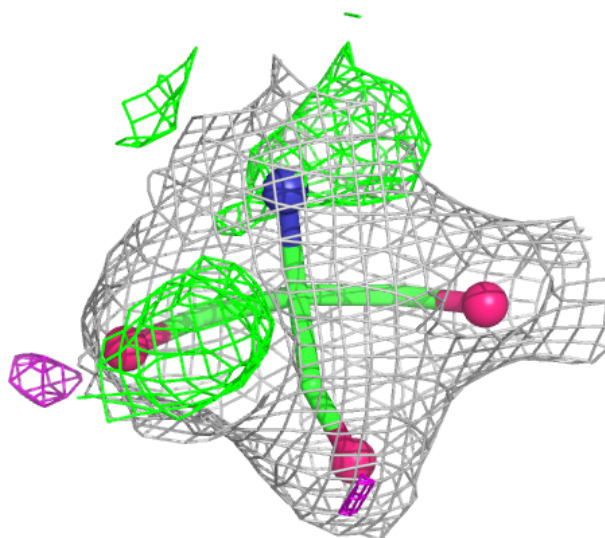
Electron density around EDO C 605:

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and green (positive)



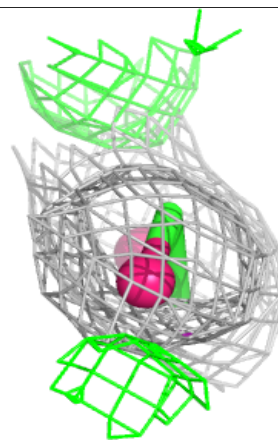
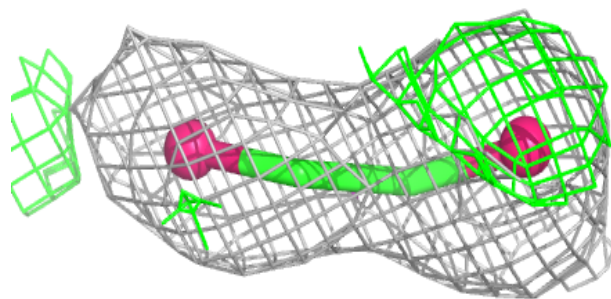
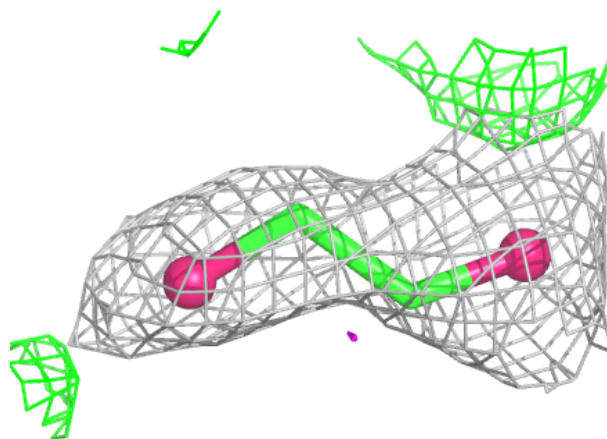
Electron density around TRS C 603:

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



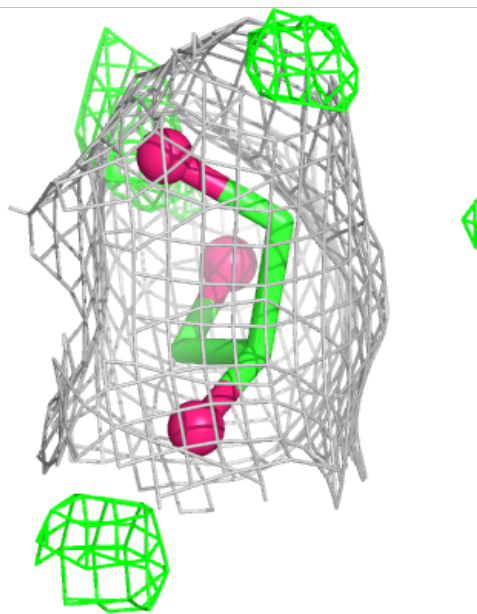
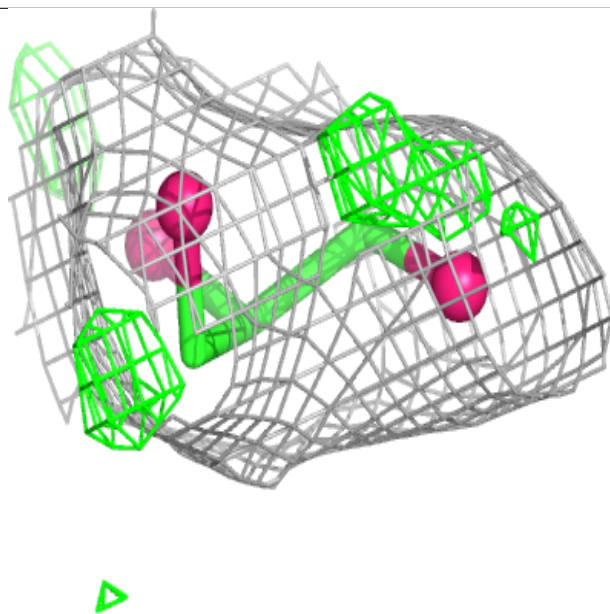
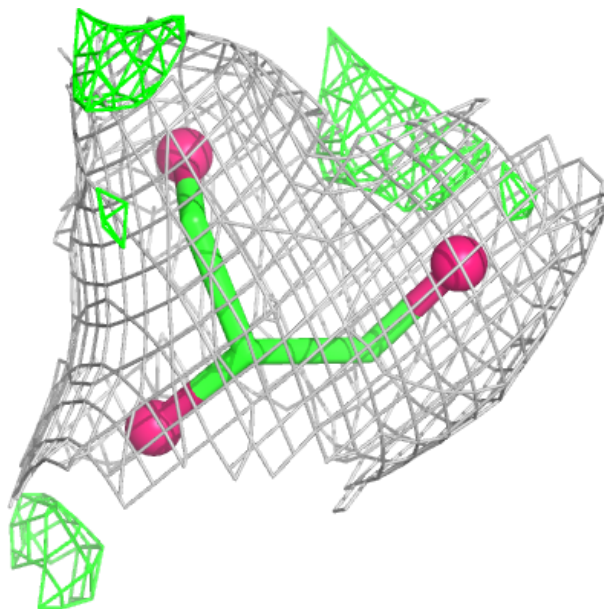
Electron density around EDO C 601:

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and green (positive)



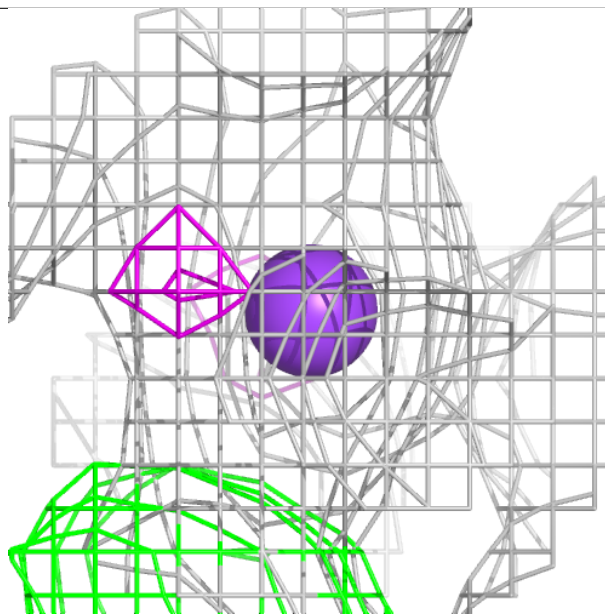
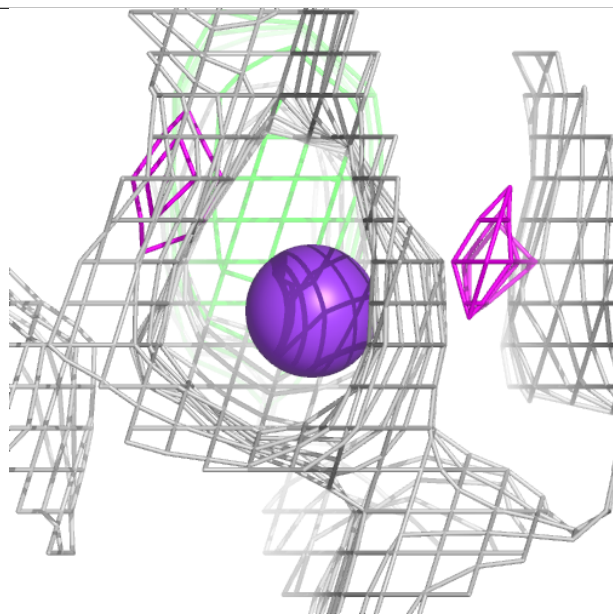
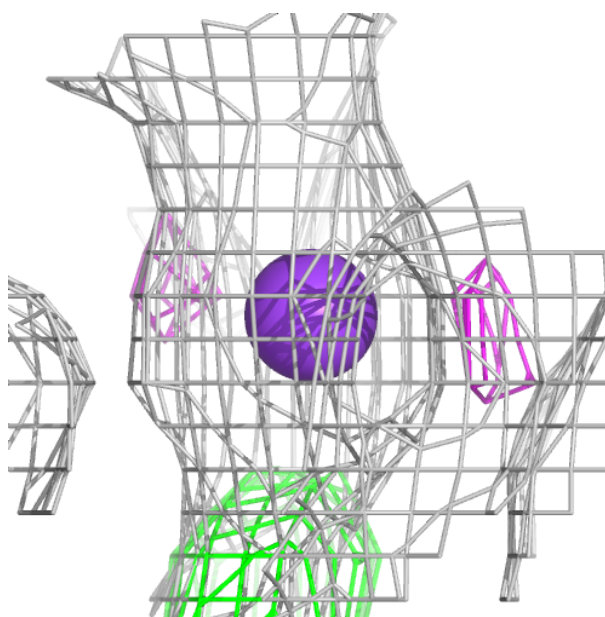
Electron density around GOL A 600:

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and green (positive)



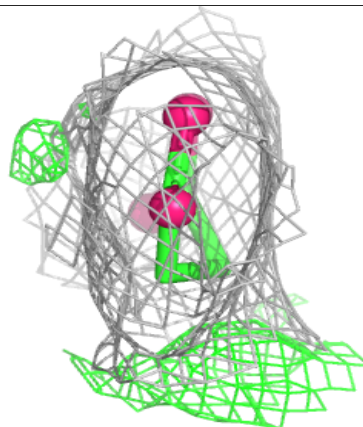
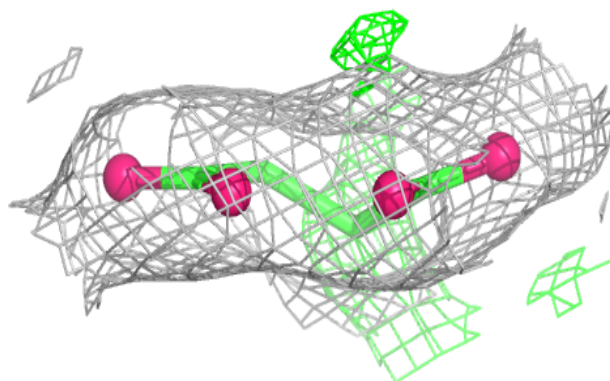
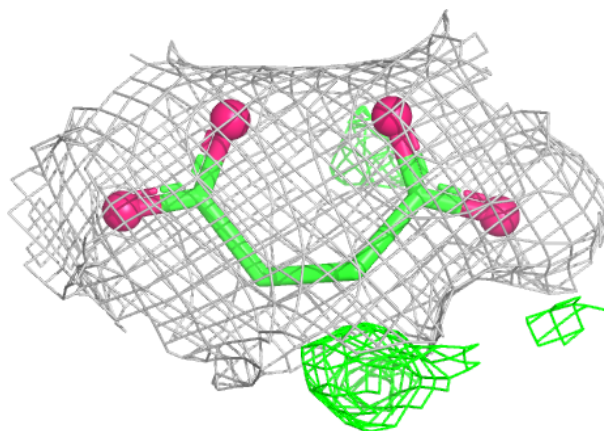
Electron density around K C 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
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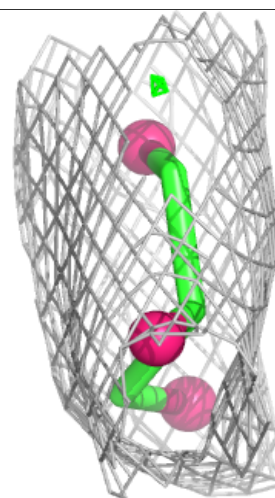
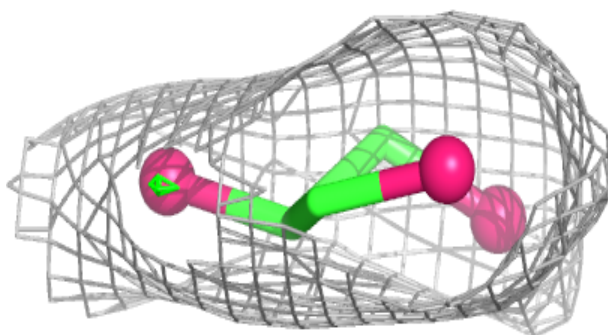
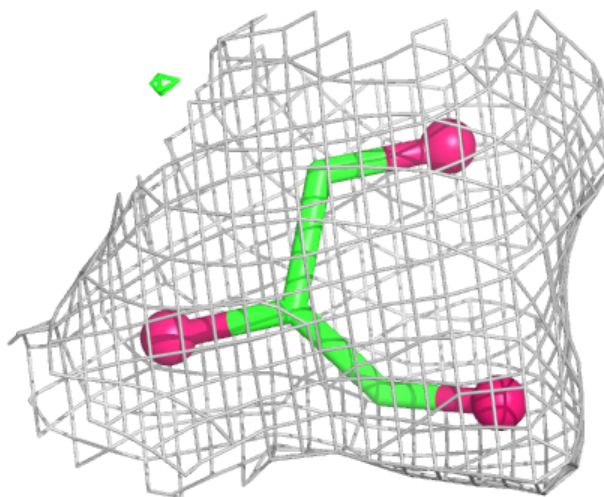
Electron density around SIN C 606:

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



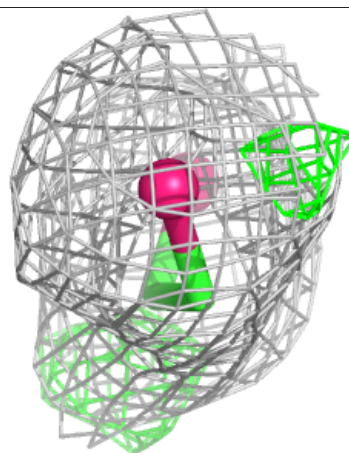
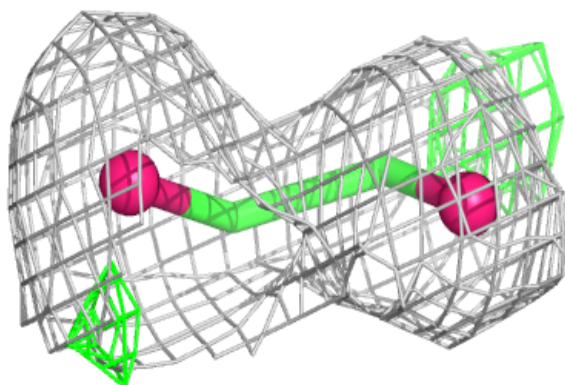
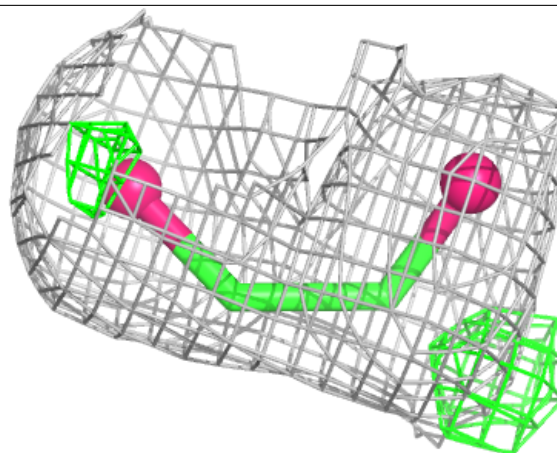
Electron density around GOL D 600:

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

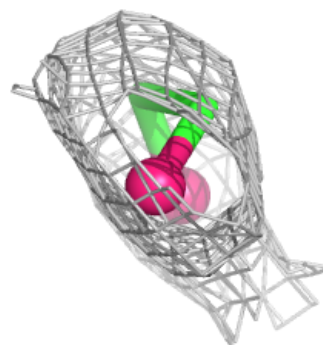
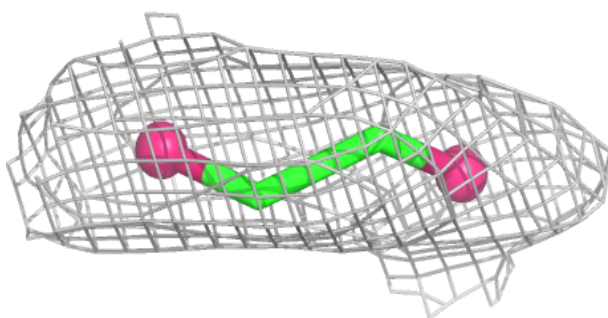
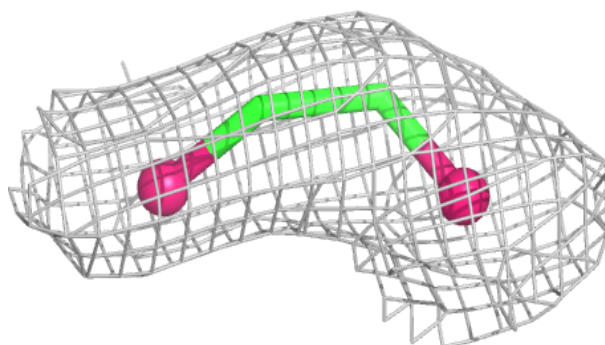


Electron density around EDO B 603:

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

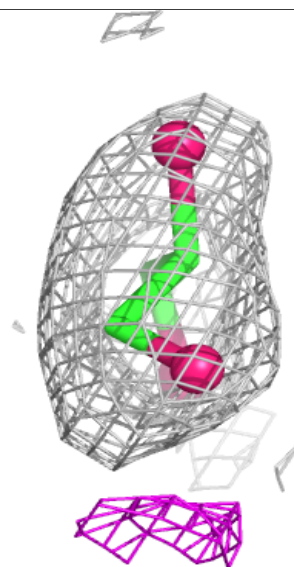
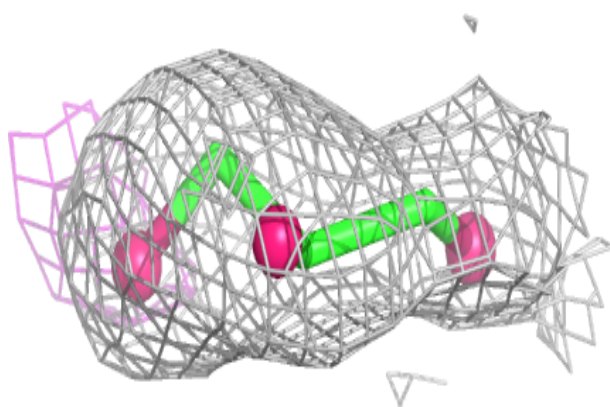
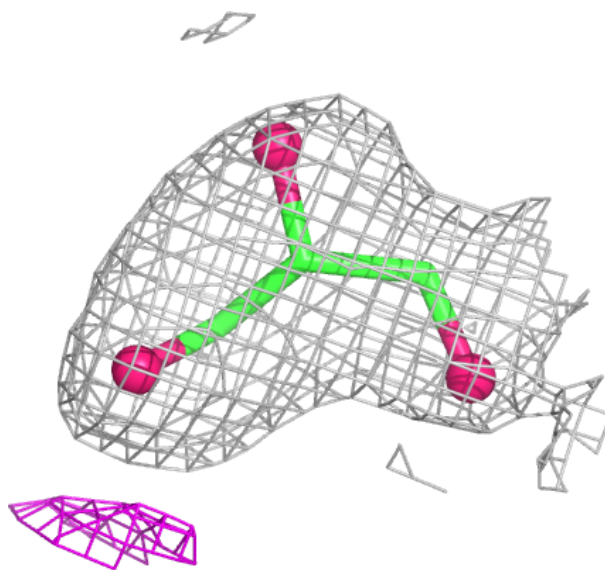
**Electron density around EDO B 602:**

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



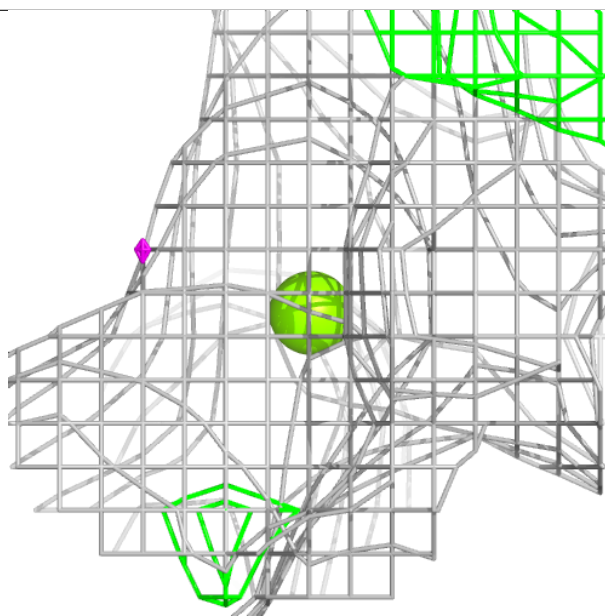
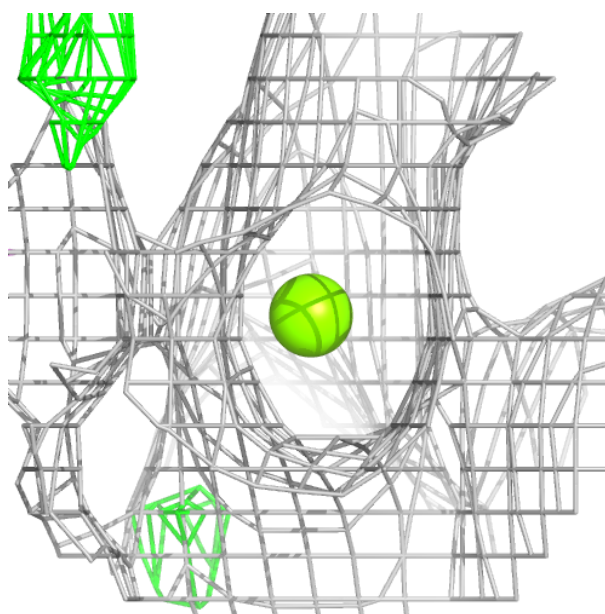
Electron density around GOL C 602:

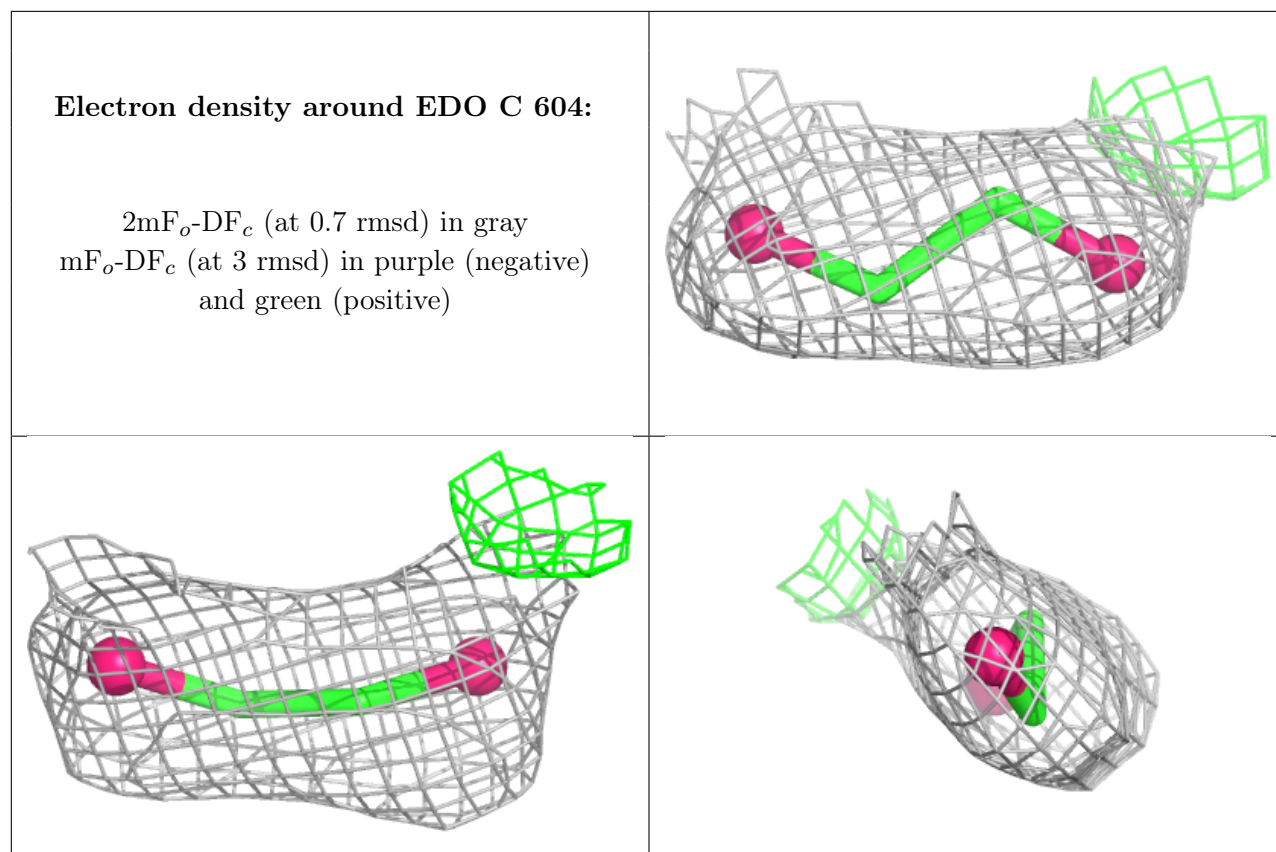
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG B 604:

$2mF_o-DF_c$ (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.