



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:50 PM EDT

PDB ID : 7KN3  
Title : Crystal structure of SARS-CoV-2 spike protein receptor-binding domain complexed with a pre-pandemic antibody S-B8 Fab  
Authors : Liu, H.; Zhu, X.; Wilson, I.A.  
Deposited on : 2020-11-04  
Resolution : 2.25 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

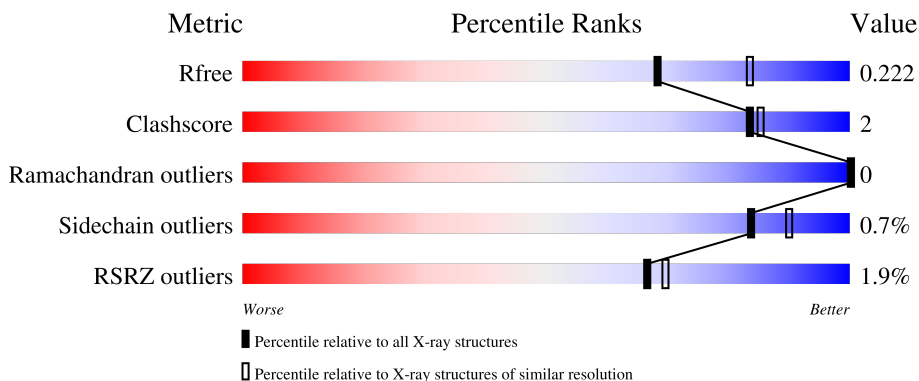
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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.



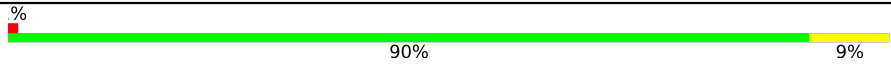
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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  $\geq 3$ , 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	231	 2% 81% 6% 16%
1	B	231	 4% 79% 6% 15%
2	H	219	 2% 94% 6%
2	M	219	 % 94% 5%
3	L	221	 93% 7%

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Mol	Chain	Length	Quality of chain
3	N	221	 <p>A horizontal bar chart representing the quality of the chain. The bar is 90% green and 9% yellow. A small red square is at the beginning of the bar. The percentage values '90%' and '9%' are printed below the bar.</p>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10195 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	194	1521	976	250	287	8	0	0	0
1	B	196	1538	985	255	290	8	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	SER	-	expression tag	UNP P0DTC2
A	543	GLY	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2
B	542	SER	-	expression tag	UNP P0DTC2
B	543	GLY	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2
B	548	HIS	-	expression tag	UNP P0DTC2
B	549	HIS	-	expression tag	UNP P0DTC2

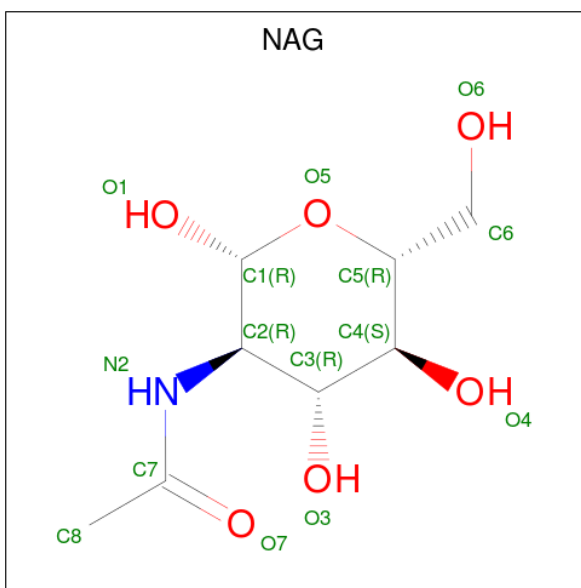
- Molecule 2 is a protein called S-B8 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	219	1619	1014	273	324	8	0	0	0
2	M	215	1590	999	267	317	7	0	0	0

- Molecule 3 is a protein called S-B8 Fab light chain.

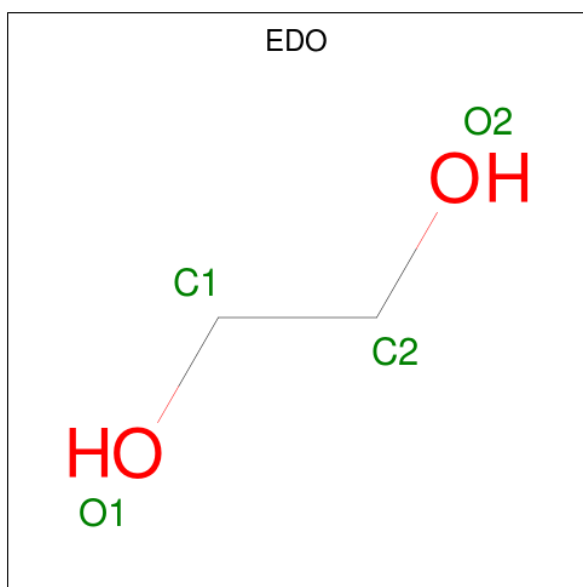
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	221	Total	C	N	O	S	0	0	0
			1693	1062	278	347	6			
3	N	221	Total	C	N	O	S	0	0	0
			1706	1070	283	347	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



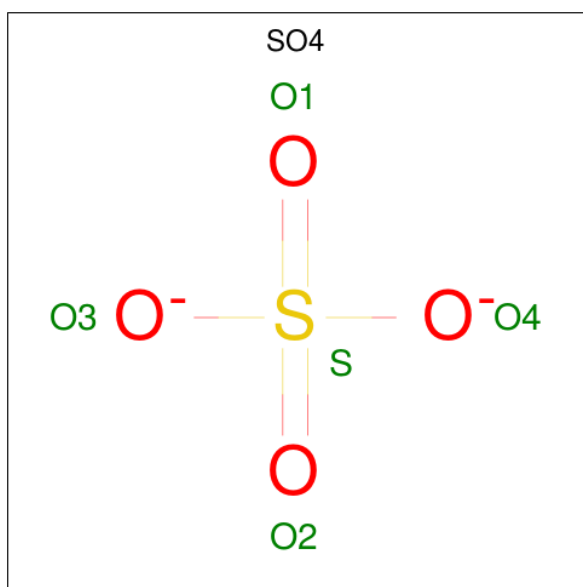
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ) (labeled as "Ligand of Interest" by depositor).



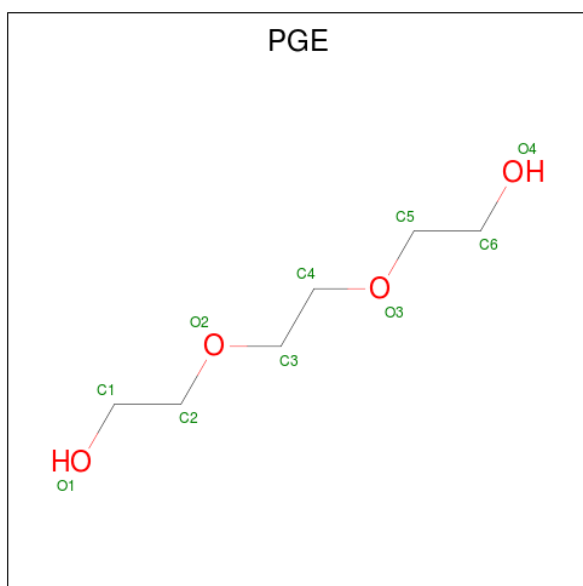
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	M	1	Total C O 4 2 2	0	0
5	N	1	Total C O 4 2 2	0	0
5	N	1	Total C O 4 2 2	0	0
5	N	1	Total C O 4 2 2	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total O S 5 4 1	0	0
6	L	1	Total O S 5 4 1	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C O 10 6 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			7	4	3		

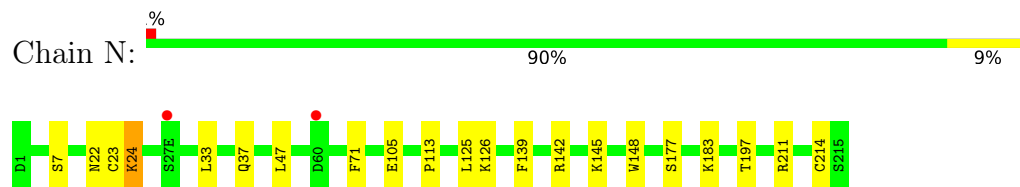
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	68	Total	O	0	0
			68	68		
8	B	43	Total	O	0	0
			43	43		
8	H	90	Total	O	0	0
			90	90		
8	L	80	Total	O	0	0
			80	80		
8	M	90	Total	O	0	0
			90	90		
8	N	70	Total	O	0	0
			70	70		





## ● Molecule 3: S-B8 Fab light chain



## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.56Å 191.56Å 117.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.91 – 2.25 47.91 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.91-2.25) 97.3 (47.91-2.25)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.24Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.186 , 0.222 0.186 , 0.222	Depositor DCC
$R_{free}$ test set	3821 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtrriage
Anisotropy	0.250	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 32.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.007 for $-1/3^*h+1/3^*k+4/3^*l,-k,2/3^*h+1/3^*k+1/3^*l$ 0.006 for $-2/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+4/3^*l,-1/3^*h+1/3^*k+1/3^*l$ 0.004 for $-h,1/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+1/3^*l$ 0.010 for $-1/3^*h-2/3^*k+4/3^*l,-2/3^*h-1/3^*k-4/3^*l,1/3^*h-1/3^*k-1/3^*l$ 0.004 for $-h,2/3^*h+1/3^*k+4/3^*l,1/3^*h+2/3^*k-1/3^*l$ 0.004 for $1/3^*h+2/3^*k-4/3^*l,-k,-2/3^*h-1/3^*k-1/3^*l$ 0.016 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10195	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, PGE, SO4, NAG

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	0.26	0/1565	0.44	0/2134
1	B	0.26	0/1581	0.43	0/2154
2	H	0.25	0/1656	0.47	0/2259
2	M	0.25	0/1626	0.46	0/2217
3	L	0.26	0/1730	0.45	0/2354
3	N	0.26	0/1743	0.44	0/2368
All	All	0.26	0/9901	0.45	0/13486

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1521	0	1411	2	0
1	B	1538	0	1440	6	0
2	H	1619	0	1559	8	0
2	M	1590	0	1529	5	0
3	L	1693	0	1621	9	0
3	N	1706	0	1656	16	0
4	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	13	0	0
5	A	8	0	12	0	0
5	H	8	0	12	0	0
5	M	4	0	6	0	0
5	N	12	0	18	1	0
6	H	5	0	0	0	0
6	L	5	0	0	0	0
7	L	17	0	23	2	0
8	A	68	0	0	0	0
8	B	43	0	0	0	0
8	H	90	0	0	0	0
8	L	80	0	0	1	0
8	M	90	0	0	1	0
8	N	70	0	0	0	0
All	All	10195	0	9313	46	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 2.

All (46) 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)
2:H:35:ASN:HD21	2:H:95:GLU:HG2	1.49	0.77
3:N:33:LEU:HD22	3:N:71:PHE:CG	2.22	0.73
3:L:142:ARG:NH1	8:L:401:HOH:O	2.22	0.72
3:L:212:GLY:H	7:L:302:PGE:H22	1.55	0.70
2:H:35:ASN:ND2	2:H:95:GLU:HG2	2.08	0.68
1:B:367:VAL:HG23	1:B:368:LEU:HD12	1.82	0.61
3:N:22:ASN:HB3	3:N:24:LYS:NZ	2.17	0.58
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.87	0.55
3:L:108:ARG:NH1	3:L:109:THR:O	2.40	0.55
8:M:467:HOH:O	3:N:214:CYS:SG	2.58	0.55
2:M:71:ARG:HB3	2:M:78:LEU:HD12	1.88	0.55
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.90	0.54
2:M:59:TYR:HB2	2:M:64:LYS:HG3	1.89	0.53
3:N:105:GLU:OE1	3:N:142:ARG:NH2	2.42	0.53
3:L:108:ARG:HD2	3:L:171:SER:HB2	1.90	0.53
3:N:148:TRP:HE1	3:N:177:SER:HG	1.57	0.53
2:M:119:PRO:HB3	2:M:145:TYR:HB3	1.90	0.53
3:L:33:LEU:HD22	3:L:71:PHE:CG	2.45	0.52
3:N:33:LEU:HD22	3:N:71:PHE:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:GLU:OE1	1:B:356:LYS:NZ	2.44	0.51
1:A:485:GLY:H	1:A:488:CYS:HB2	1.77	0.50
1:B:431:GLY:HA2	1:B:515:PHE:CD2	2.47	0.49
3:N:145:LYS:HB3	3:N:197:THR:HB	1.94	0.49
3:L:113:PRO:HB3	3:L:139:PHE:HB3	1.95	0.49
3:N:22:ASN:HB3	3:N:24:LYS:HZ1	1.76	0.49
3:N:113:PRO:HB3	3:N:139:PHE:HB3	1.96	0.48
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.48	0.48
3:N:23:CYS:C	3:N:24:LYS:HD3	2.34	0.48
3:L:190:LYS:HD2	3:L:210:ASN:HB3	1.96	0.47
3:N:211:ARG:HH22	5:N:302:EDO:H21	1.78	0.47
1:B:379:CYS:HA	1:B:432:CYS:HA	1.98	0.45
3:N:126:LYS:HA	3:N:126:LYS:HD2	1.71	0.45
1:B:378:LYS:HG2	1:B:380:TYR:CZ	2.52	0.45
2:H:193:THR:HG23	2:H:210:LYS:HE2	1.99	0.45
3:N:22:ASN:CB	3:N:24:LYS:NZ	2.81	0.44
3:N:125:LEU:O	3:N:183:LYS:HD2	2.15	0.44
2:H:216:CYS:HB3	3:L:214:CYS:HB2	1.77	0.44
7:L:302:PGE:H2	7:L:302:PGE:H52	2.00	0.43
2:H:142:VAL:HG11	2:H:150:VAL:HG11	2.00	0.42
2:M:165:THR:HG23	2:M:178:LEU:HD21	2.01	0.42
2:M:35:ASN:ND2	2:M:95:GLU:OE1	2.51	0.42
3:L:13:VAL:HB	3:L:78:LEU:HD22	2.01	0.42
1:B:392:PHE:HD1	1:B:517:LEU:HG	1.85	0.42
2:H:94:ARG:O	2:H:100:MET:HA	2.20	0.41
3:N:125:LEU:HD23	3:N:125:LEU:HA	1.90	0.41
2:H:196:CYS:SG	2:H:209:LYS:HB3	2.61	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	192/231 (83%)	187 (97%)	5 (3%)	0	100	100
1	B	194/231 (84%)	187 (96%)	7 (4%)	0	100	100
2	H	217/219 (99%)	214 (99%)	3 (1%)	0	100	100
2	M	211/219 (96%)	209 (99%)	2 (1%)	0	100	100
3	L	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
3	N	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
All	All	1252/1342 (93%)	1227 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	162/203 (80%)	160 (99%)	2 (1%)	71	80
1	B	165/203 (81%)	164 (99%)	1 (1%)	86	91
2	H	180/184 (98%)	179 (99%)	1 (1%)	86	91
2	M	175/184 (95%)	175 (100%)	0	100	100
3	L	191/195 (98%)	190 (100%)	1 (0%)	88	92
3	N	195/195 (100%)	193 (99%)	2 (1%)	76	84
All	All	1068/1164 (92%)	1061 (99%)	7 (1%)	84	90

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

Mol	Chain	Res	Type
1	A	377	PHE
1	A	386	LYS
1	B	375	SER
2	H	206	LYS
3	L	46	LEU
3	N	7	SER
3	N	24	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	35	ASN
2	M	3	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	1001	1	14,14,15	0.69	1 (7%)	17,19,21	0.94	1 (5%)
6	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.05	0
5	EDO	A	1002	-	3,3,3	0.45	0	2,2,2	0.36	0
7	PGE	L	302	-	9,9,9	0.30	0	8,8,8	0.32	0
5	EDO	H	303	-	3,3,3	0.47	0	2,2,2	0.30	0
6	SO4	H	301	-	4,4,4	0.14	0	6,6,6	0.04	0
5	EDO	N	301	-	3,3,3	0.45	0	2,2,2	0.33	0
7	PGE	L	303	-	6,6,9	0.27	0	5,5,8	0.32	0
5	EDO	H	302	-	3,3,3	0.44	0	2,2,2	0.39	0
5	EDO	N	303	-	3,3,3	0.46	0	2,2,2	0.32	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	N	302	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	M	301	-	3,3,3	0.46	0	2,2,2	0.30	0
5	EDO	A	1003	-	3,3,3	0.44	0	2,2,2	0.34	0
4	NAG	B	1001	1	14,14,15	0.34	0	17,19,21	0.44	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
4	NAG	A	1001	1	-	1/6/23/26	0/1/1/1
5	EDO	A	1002	-	-	0/1/1/1	-
7	PGE	L	302	-	-	4/7/7/7	-
5	EDO	H	303	-	-	0/1/1/1	-
5	EDO	N	301	-	-	0/1/1/1	-
7	PGE	L	303	-	-	2/4/4/7	-
5	EDO	H	302	-	-	0/1/1/1	-
5	EDO	N	303	-	-	0/1/1/1	-
5	EDO	N	302	-	-	0/1/1/1	-
5	EDO	M	301	-	-	0/1/1/1	-
5	EDO	A	1003	-	-	0/1/1/1	-
4	NAG	B	1001	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	NAG	O5-C1	-2.42	1.39	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	NAG	C1-O5-C5	2.62	115.74	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	302	PGE	O2-C3-C4-O3
7	L	302	PGE	C3-C4-O3-C5

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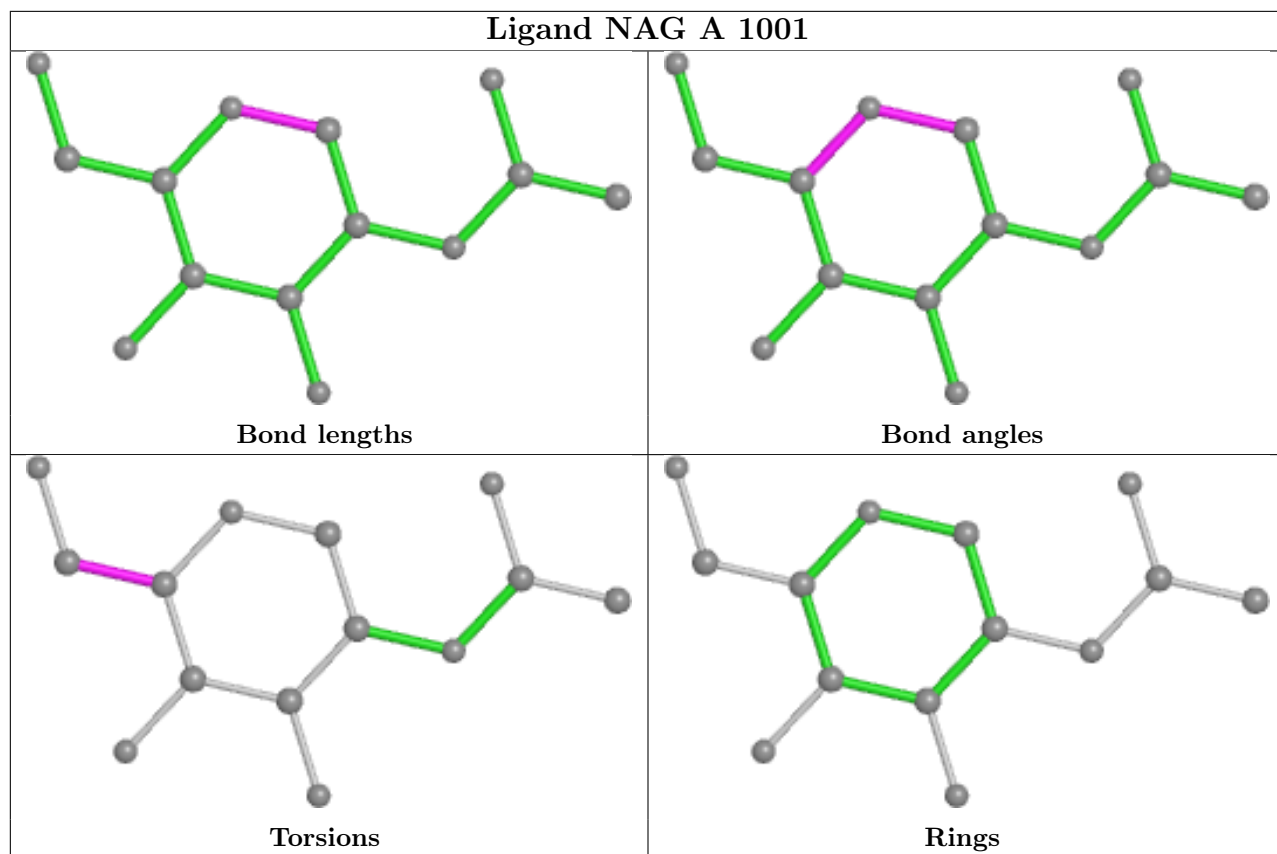
Mol	Chain	Res	Type	Atoms
4	A	1001	NAG	O5-C5-C6-O6
4	B	1001	NAG	O5-C5-C6-O6
7	L	303	PGE	O2-C3-C4-O3
4	B	1001	NAG	C4-C5-C6-O6
7	L	302	PGE	O1-C1-C2-O2
7	L	303	PGE	C1-C2-O2-C3
7	L	302	PGE	C4-C3-O2-C2

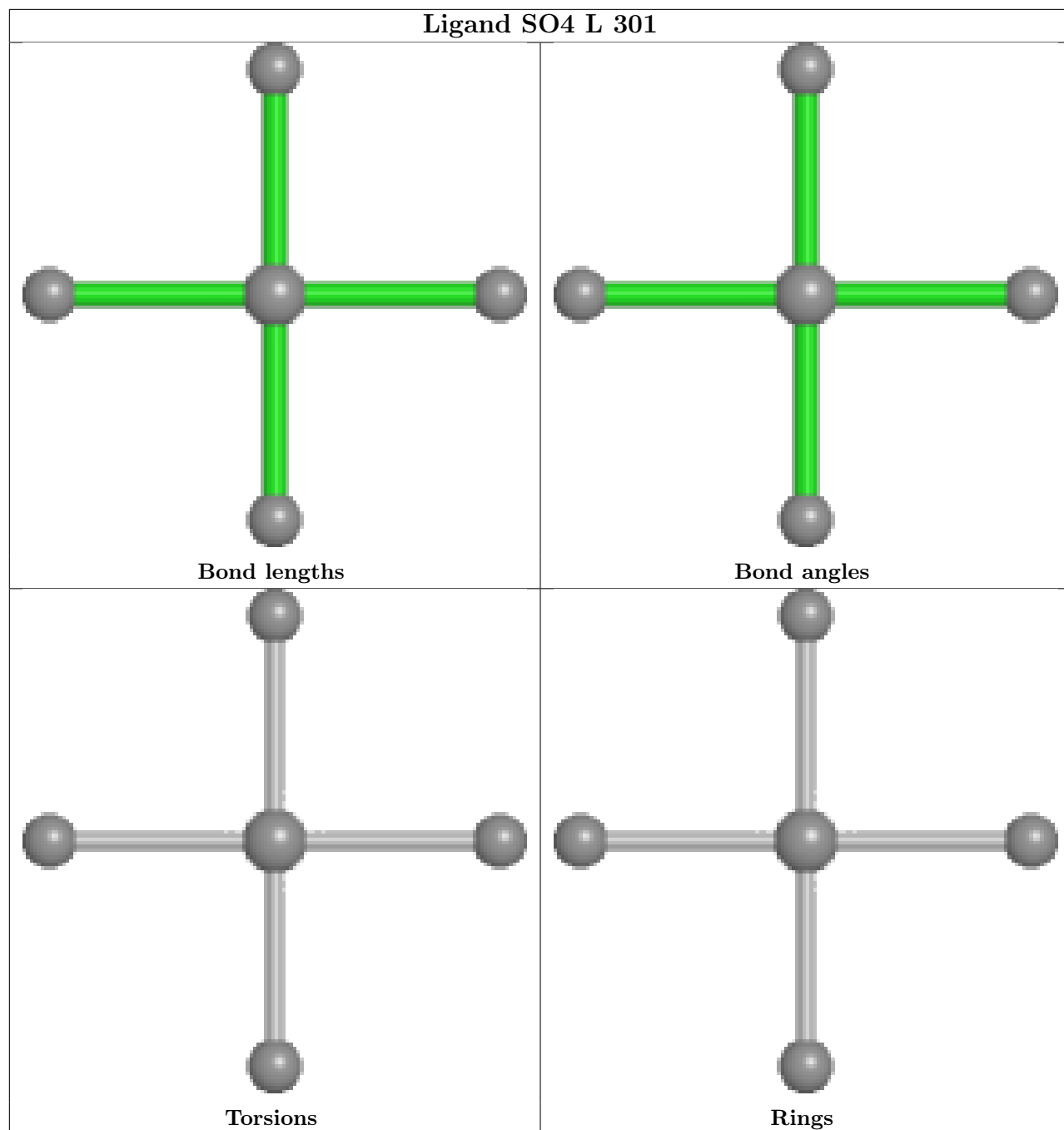
There are no ring outliers.

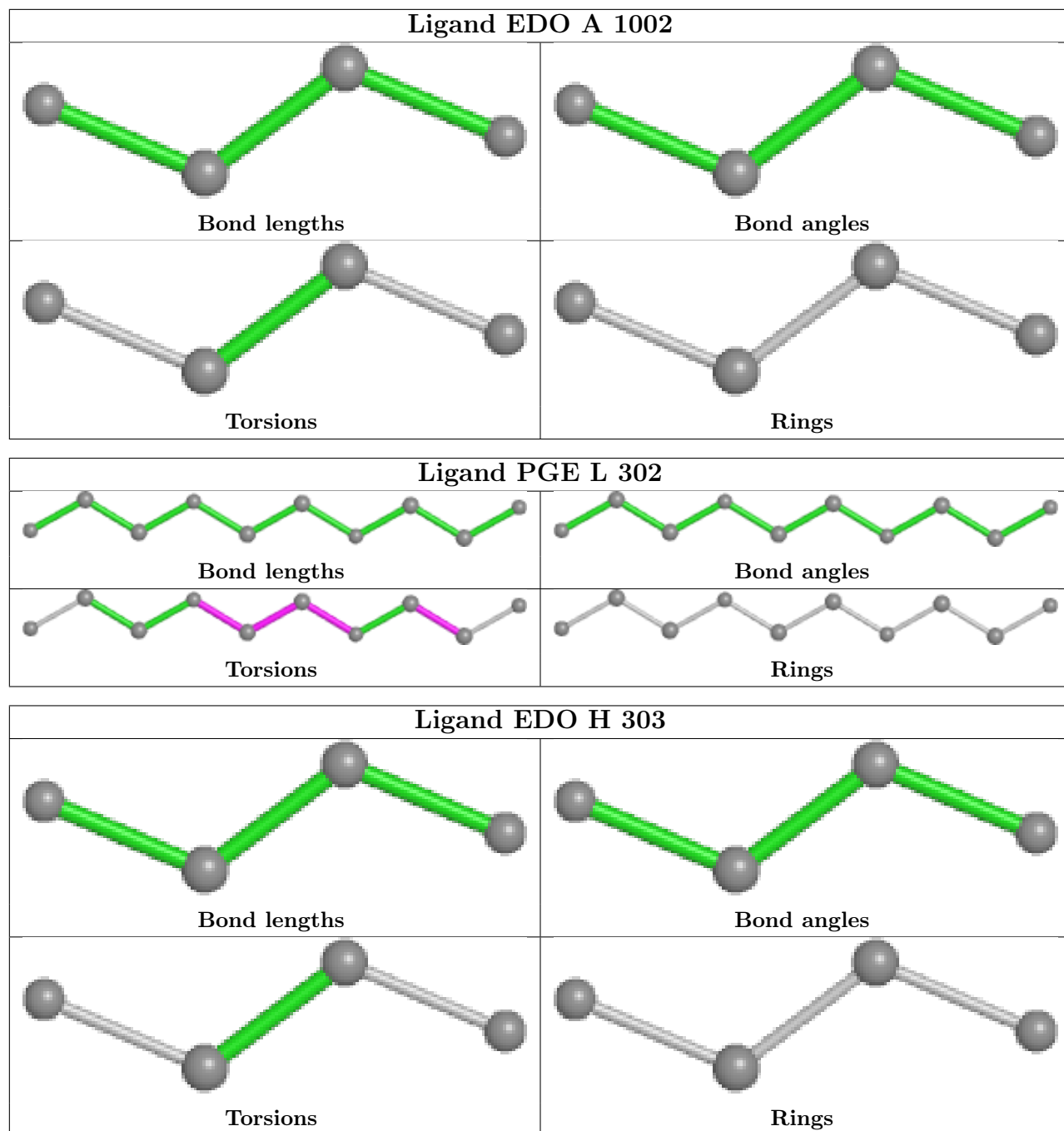
2 monomers are involved in 3 short contacts:

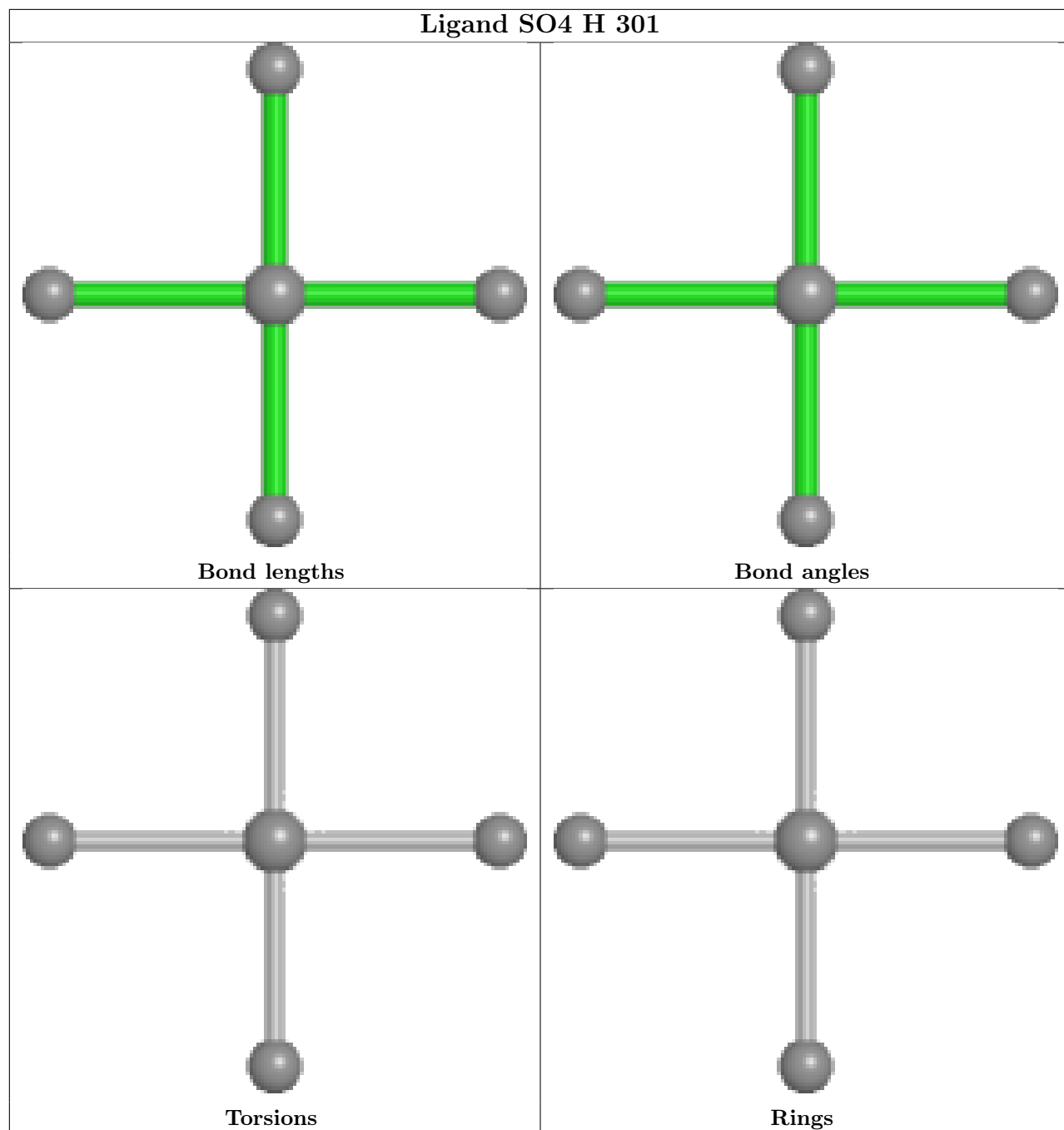
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	302	PGE	2	0
5	N	302	EDO	1	0

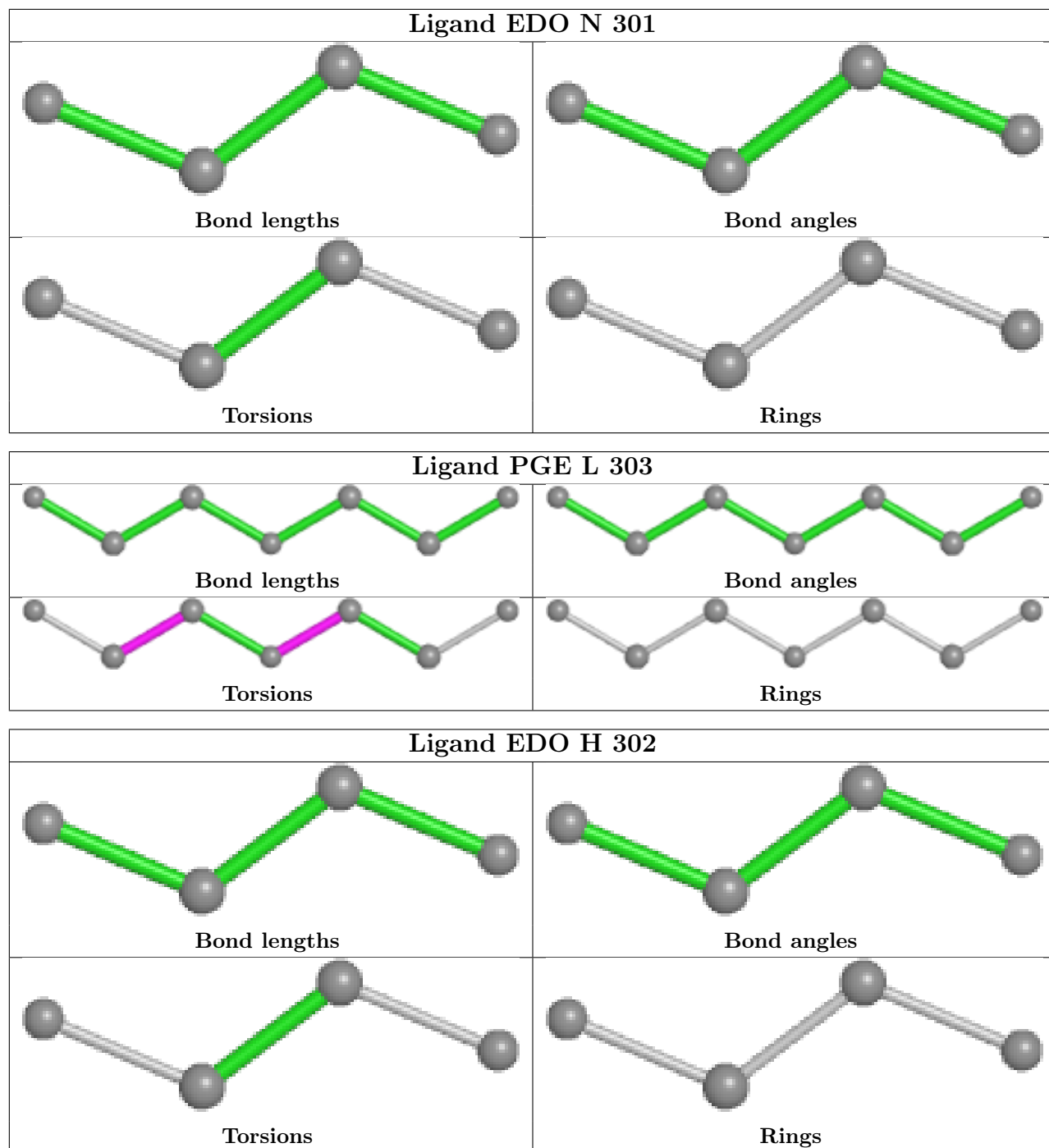
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

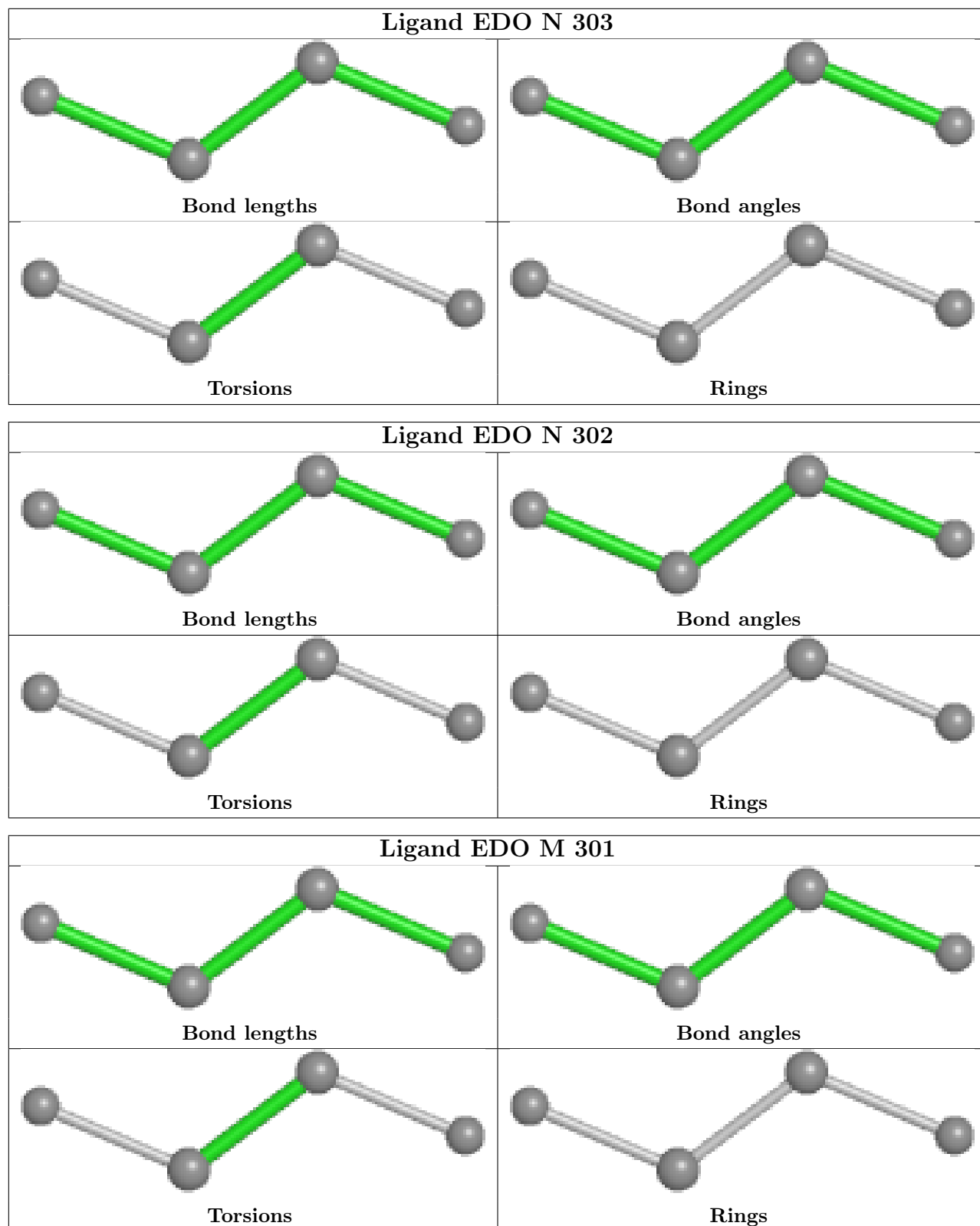




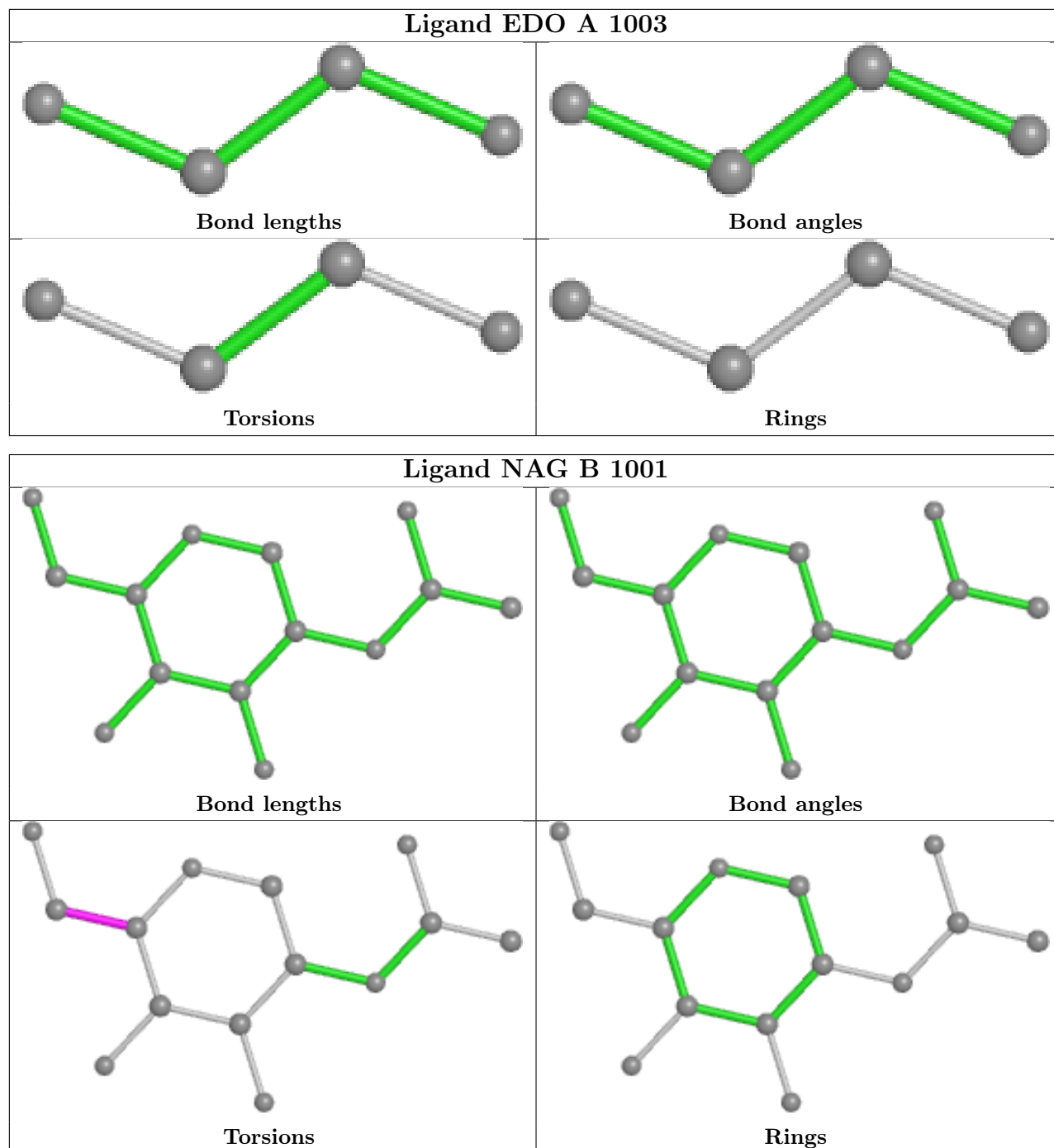












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	194/231 (83%)	0.06	4 (2%) 63 66	22, 41, 68, 82	0
1	B	196/231 (84%)	0.23	10 (5%) 28 30	30, 46, 78, 90	0
2	H	219/219 (100%)	-0.11	5 (2%) 60 63	25, 35, 56, 102	0
2	M	215/219 (98%)	-0.17	2 (0%) 84 85	25, 39, 56, 74	0
3	L	221/221 (100%)	-0.10	1 (0%) 91 91	25, 41, 59, 75	0
3	N	221/221 (100%)	-0.09	2 (0%) 84 85	24, 42, 60, 71	0
All	All	1266/1342 (94%)	-0.04	24 (1%) 66 69	22, 40, 66, 102	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	216	CYS	4.7
1	B	372	ALA	4.4
1	B	333	THR	3.9
1	B	477	SER	3.8
1	B	369	TYR	3.0
2	H	130	SER	3.0
1	B	519	HIS	3.0
1	A	369	TYR	2.9
2	H	131	THR	2.7
1	B	520	ALA	2.6
1	B	334	ASN	2.6
1	B	505	TYR	2.6
1	B	370	ASN	2.6
3	N	60	ASP	2.5
2	M	133	GLY	2.5
2	M	215	SER	2.5
3	L	214	CYS	2.5
1	A	366	SER	2.4
1	A	334	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	215	SER	2.2
3	N	27(E)	SER	2.2
1	B	373	SER	2.1
1	A	525	CYS	2.1
2	H	133	GLY	2.1

## 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

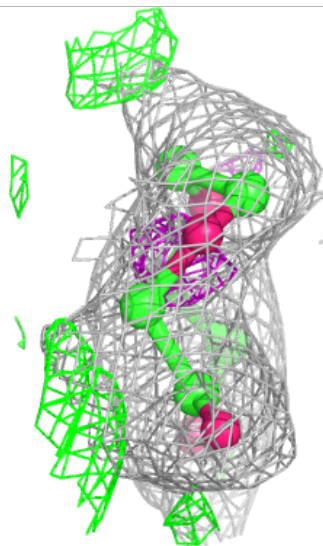
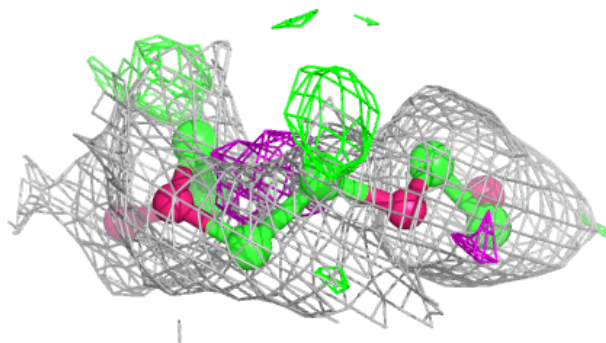
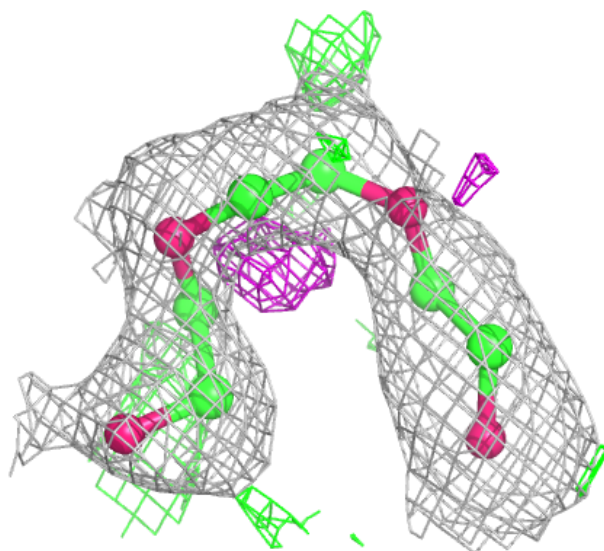
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	PGE	L	302	10/10	0.59	0.22	58,68,73,73	0
4	NAG	B	1001	14/15	0.78	0.28	50,58,67,67	0
5	EDO	N	303	4/4	0.81	0.17	51,51,52,53	0
6	SO4	L	301	5/5	0.85	0.14	100,100,101,104	0
7	PGE	L	303	7/10	0.85	0.24	68,71,72,72	0
5	EDO	H	303	4/4	0.87	0.17	39,39,43,43	0
5	EDO	M	301	4/4	0.87	0.15	37,41,41,43	0
4	NAG	A	1001	14/15	0.87	0.26	59,70,75,75	0
5	EDO	N	302	4/4	0.90	0.11	64,65,65,66	0
5	EDO	N	301	4/4	0.93	0.29	43,43,44,45	0
5	EDO	A	1003	4/4	0.94	0.15	50,51,53,54	0
5	EDO	A	1002	4/4	0.96	0.12	37,39,40,44	0
5	EDO	H	302	4/4	0.97	0.18	38,39,41,46	0
6	SO4	H	301	5/5	0.99	0.14	56,56,58,61	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

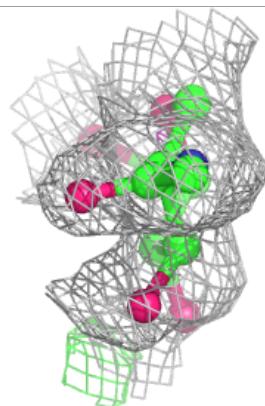
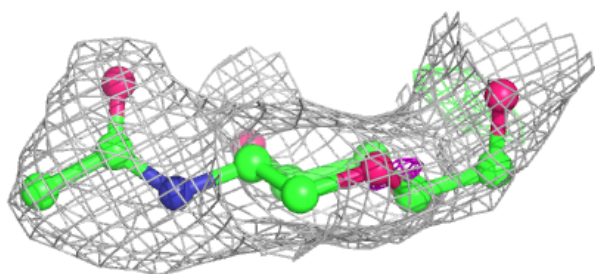
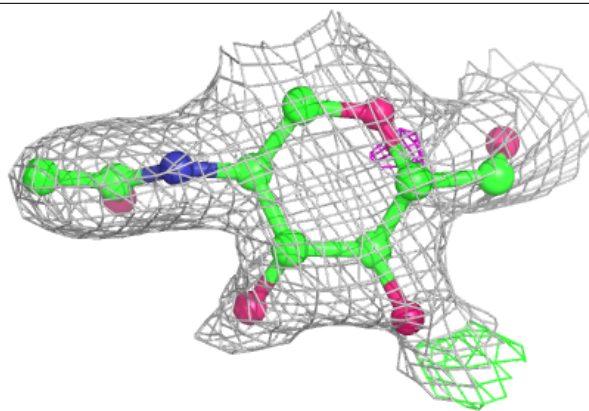
**Electron density around PGE L 302:**

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

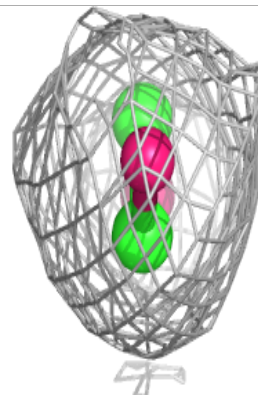
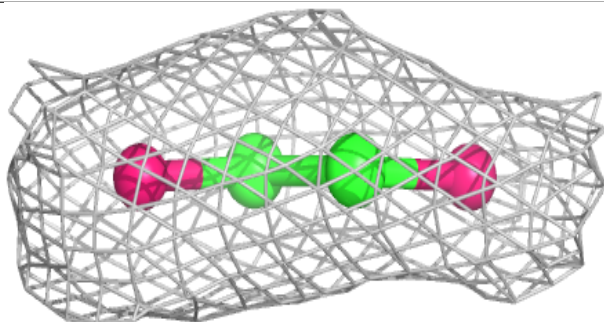
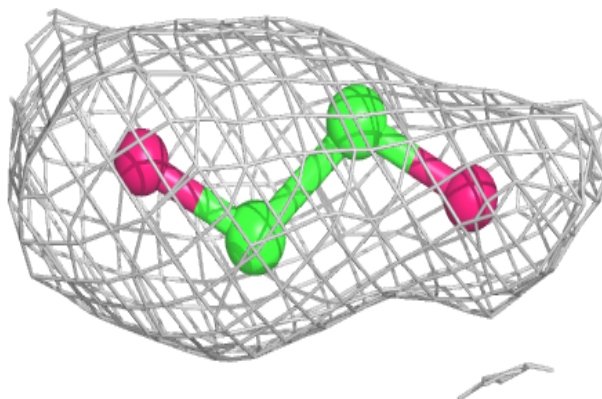


**Electron density around NAG B 1001:**

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

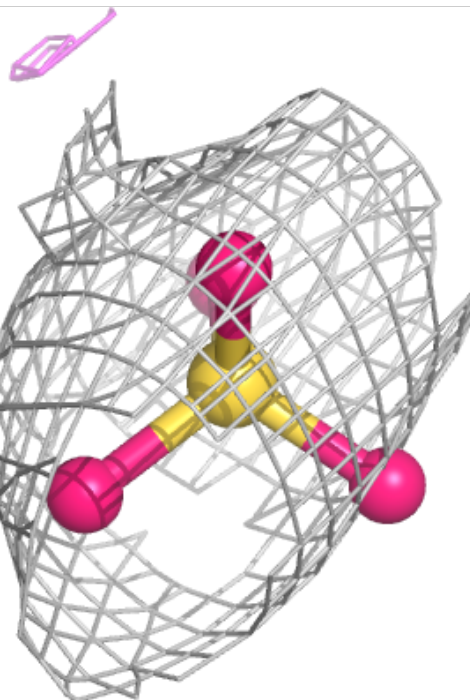
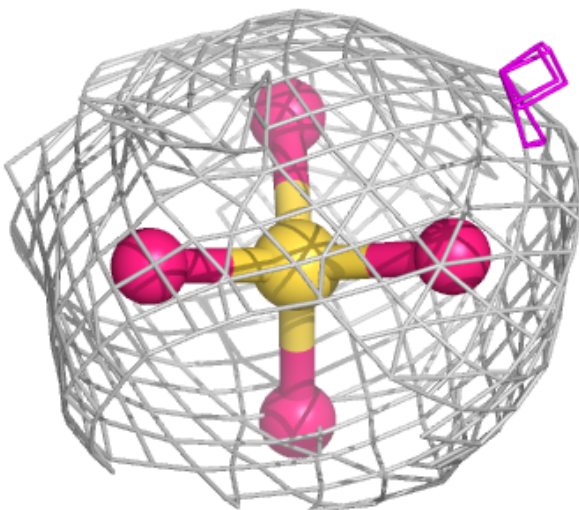
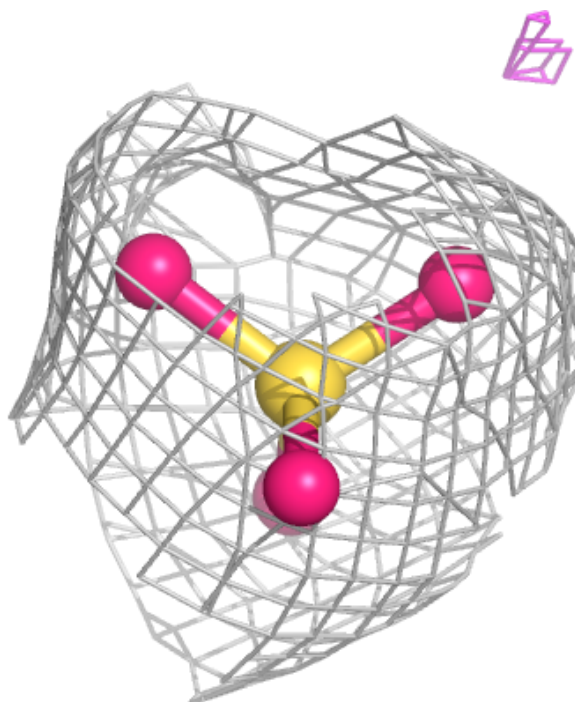
**Electron density around EDO N 303:**

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

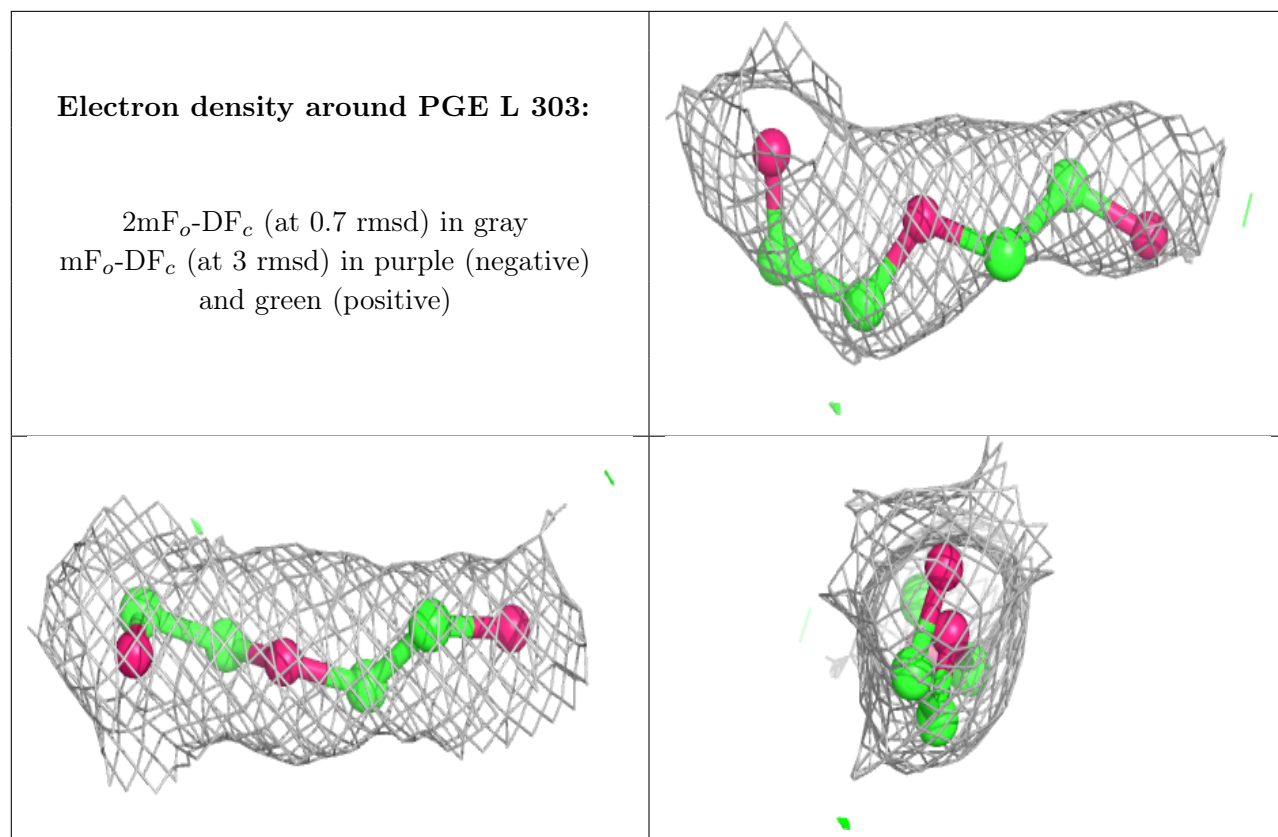


**Electron density around SO4 L 301:**

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and green (positive)

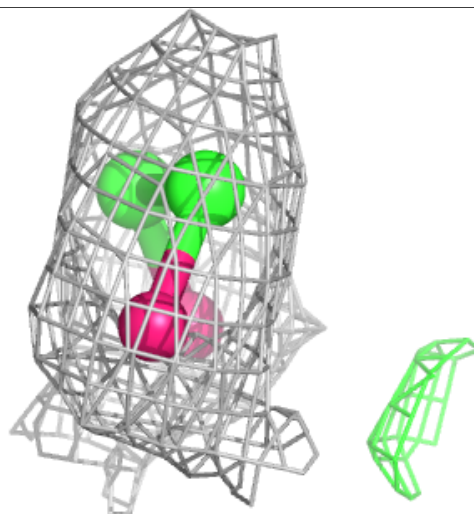
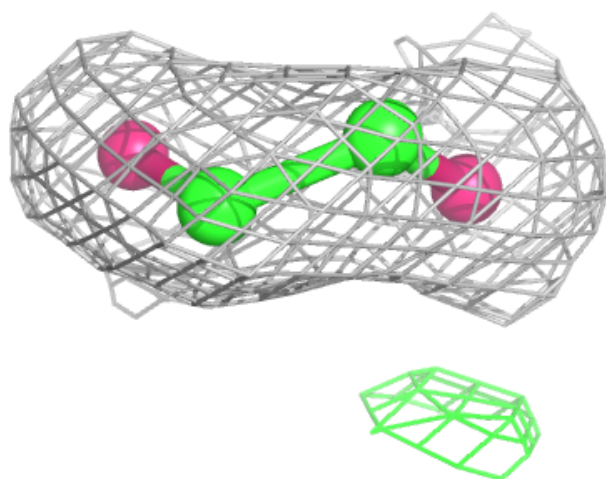
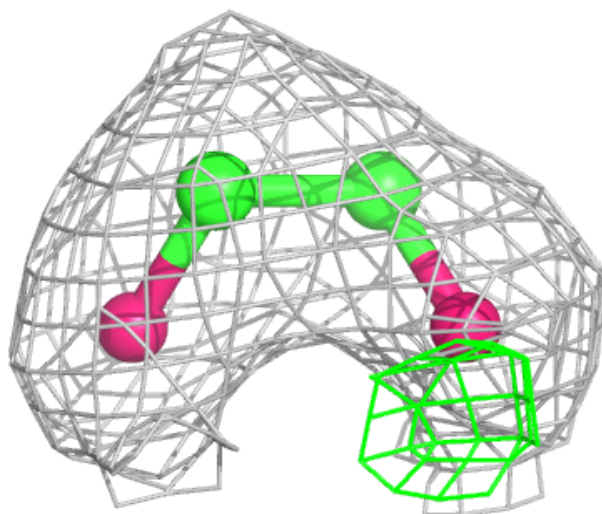






**Electron density around EDO H 303:**

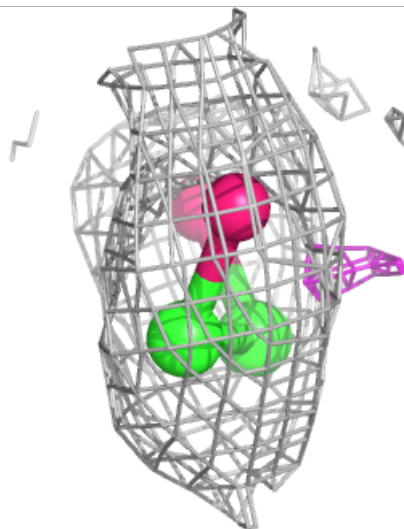
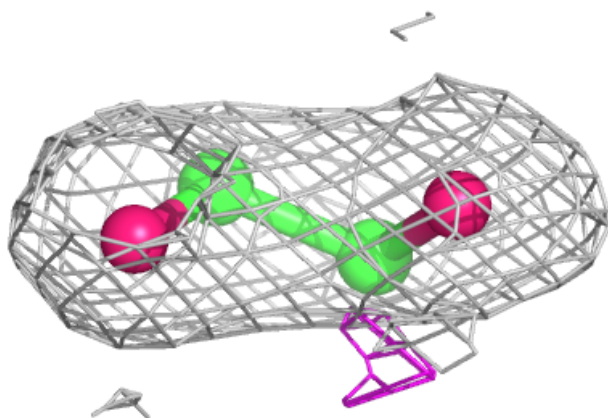
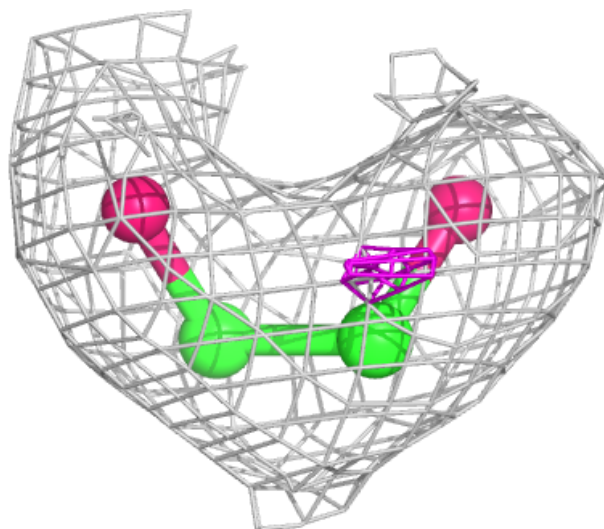
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





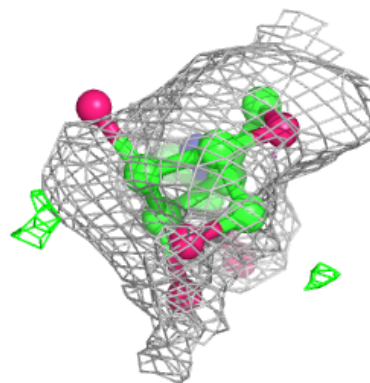
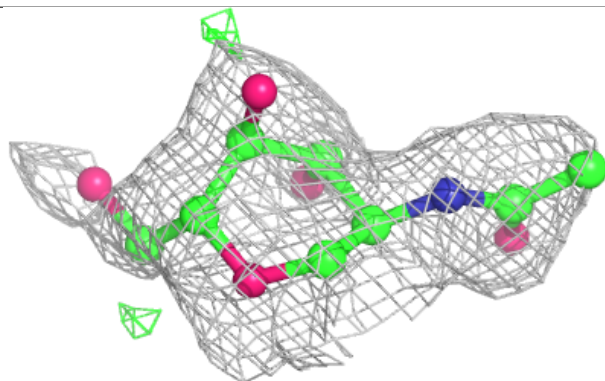
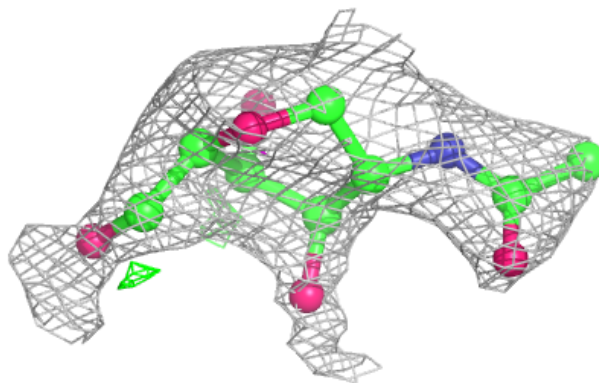
**Electron density around EDO M 301:**

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and green (positive)

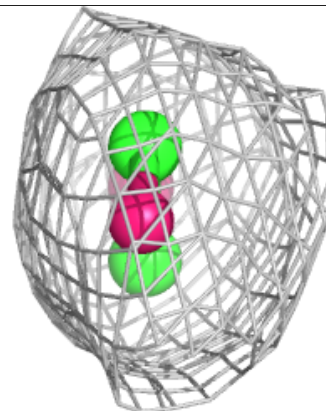
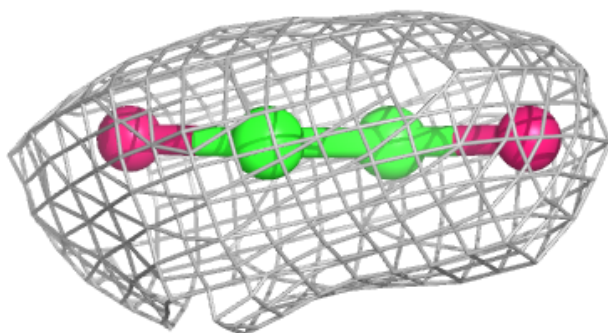
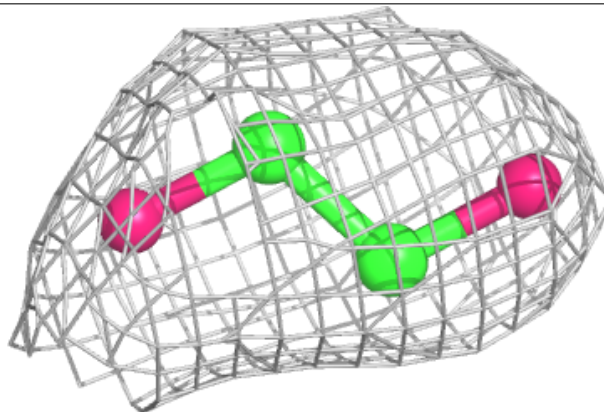


**Electron density around NAG A 1001:**

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

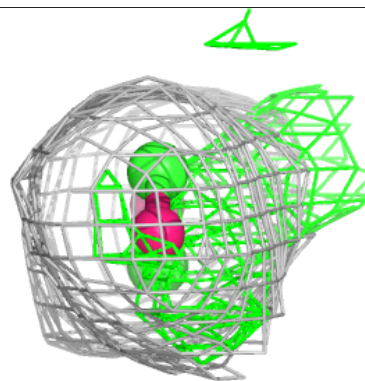
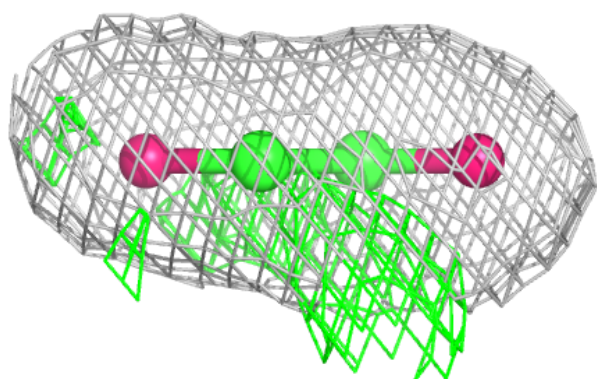
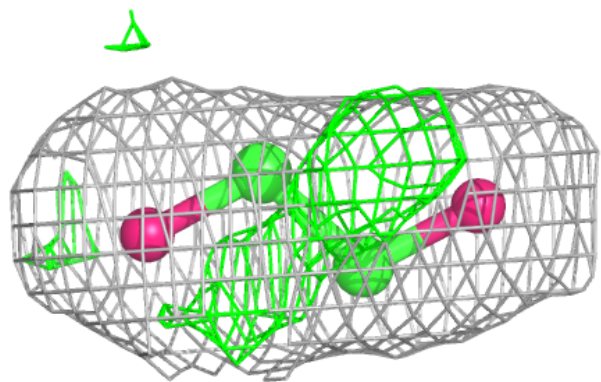
**Electron density around EDO N 302:**

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and green (positive)



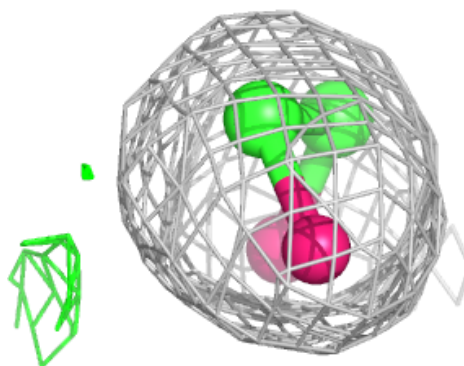
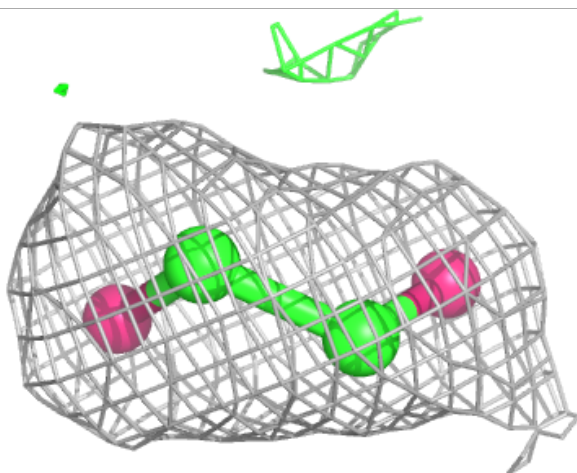
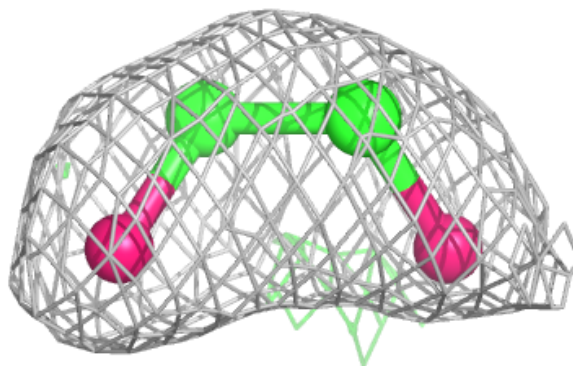
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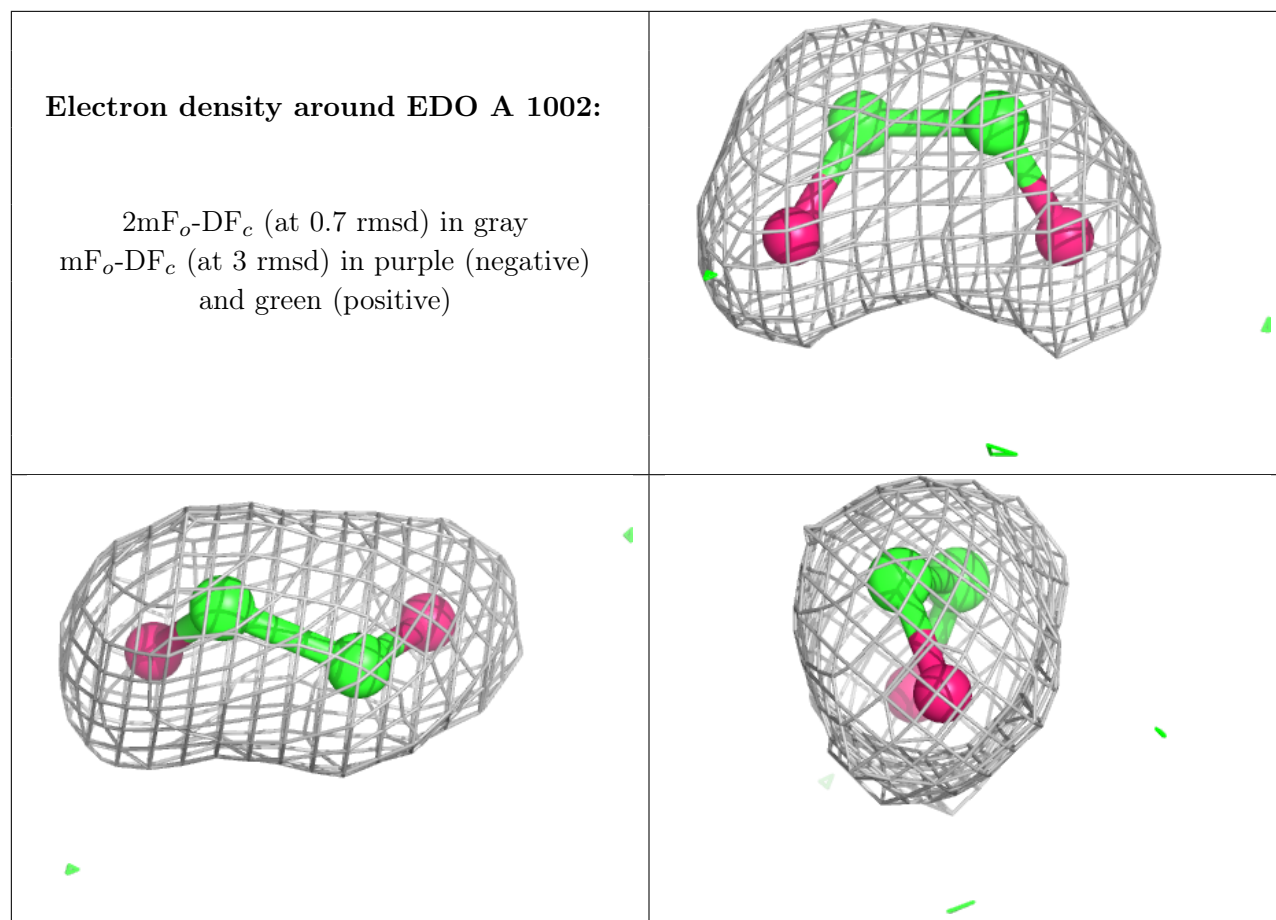
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around EDO A 1003:**

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

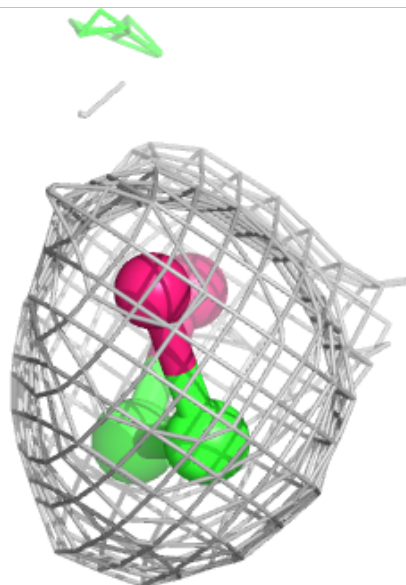
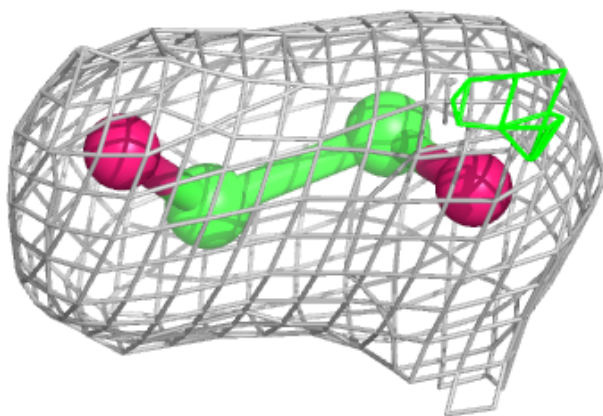
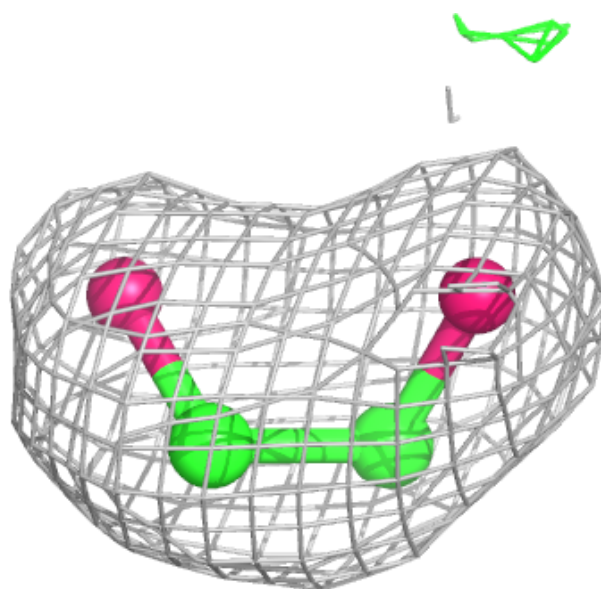


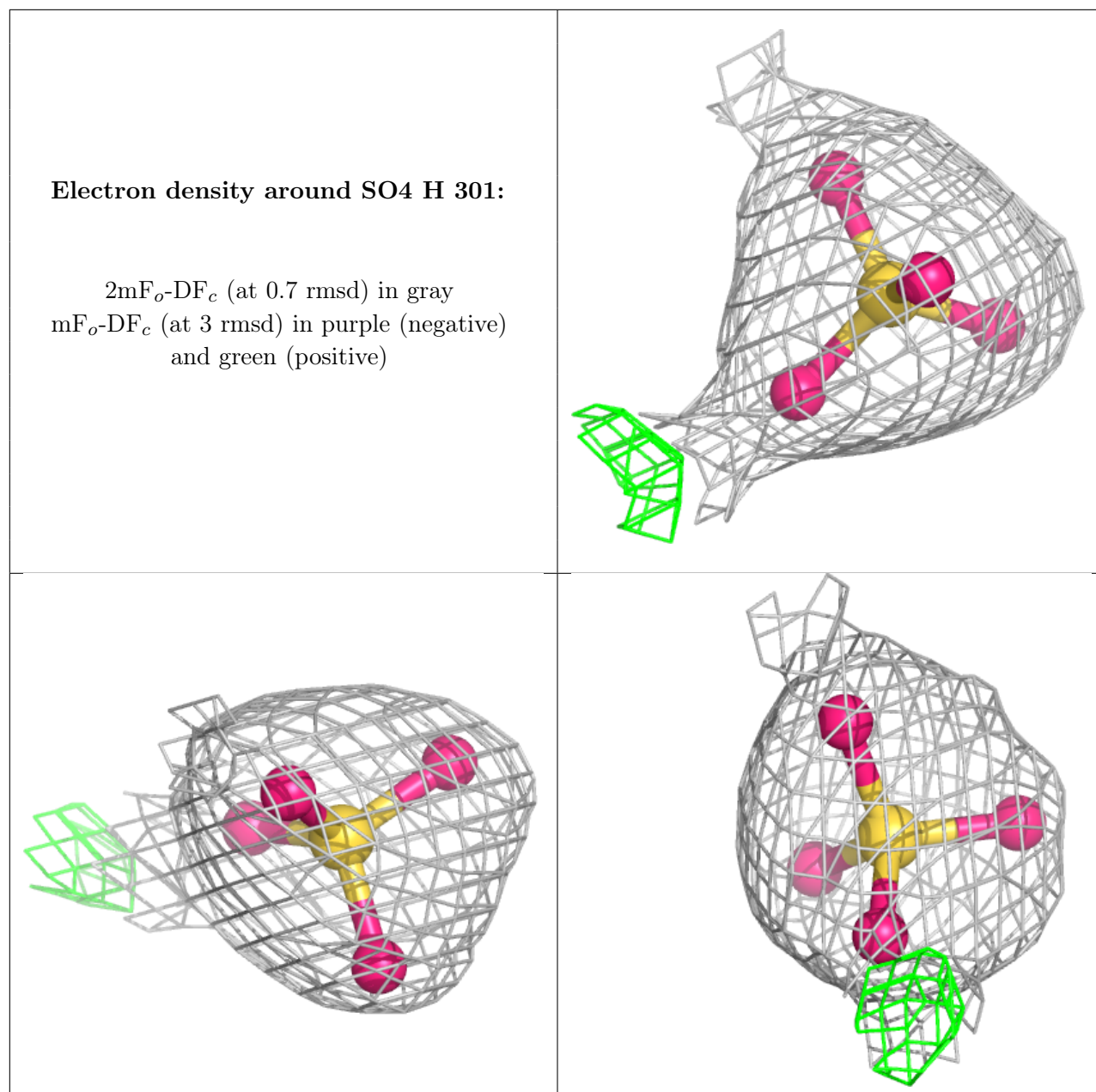




**Electron density around EDO H 302:**

$2mF_o-DF_c$  (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.