



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 10:30 PM EDT

PDB ID : 6ASQ  
Title : Structure of Grp94 bound to methyl 2-[2-(2-benzylpyridin-3-yl)ethyl]-3-chloro-4,6-dihydroxybenzoate, a pan-Hsp90 inhibitor  
Authors : Huard, D.J.E.; Lieberman, R.L.  
Deposited on : 2017-08-25  
Resolution : 2.35 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

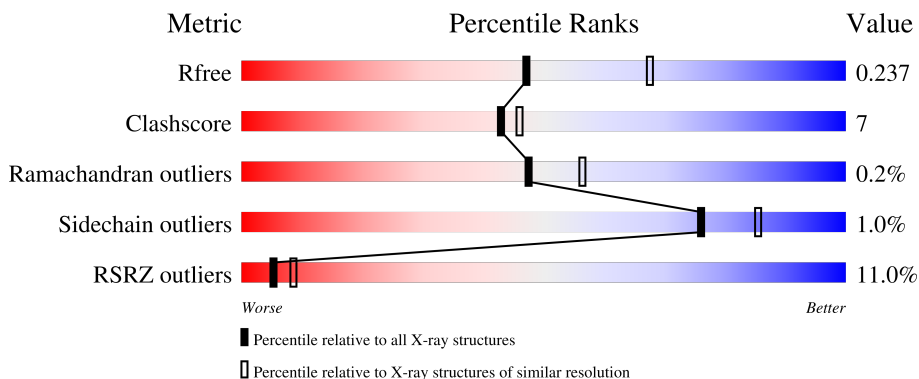
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	233	
1	B	233	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3737 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.

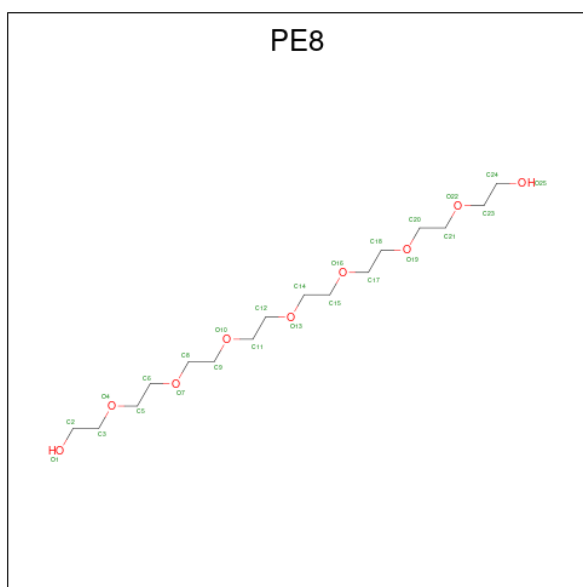
- Molecule 1 is a protein called Endoplasmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	1713	1091	285	331	6	0	0	0
1	B	218	1728	1098	285	339	6	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SER	-	expression tag	UNP P41148
A	324	GLY	-	linker	UNP P41148
A	325	GLY	-	linker	UNP P41148
A	326	GLY	-	linker	UNP P41148
A	327	GLY	-	linker	UNP P41148
B	68	SER	-	expression tag	UNP P41148
B	324	GLY	-	linker	UNP P41148
B	325	GLY	-	linker	UNP P41148
B	326	GLY	-	linker	UNP P41148
B	327	GLY	-	linker	UNP P41148

- Molecule 2 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>9</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 25 16 9	0	0
2	A	1	Total C O 13 8 5	0	0
2	A	1	Total C O 16 10 6	0	0
2	A	1	Total C O 13 8 5	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 16 10 6	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 6 4 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



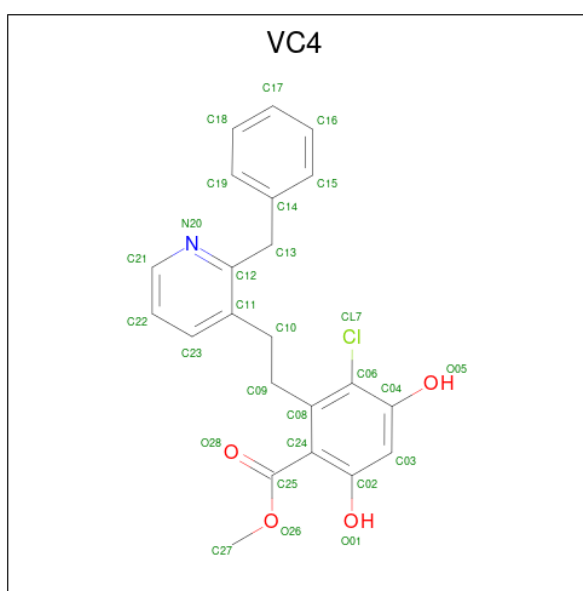
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is methyl 2-[2-(2-benzylpyridin-3-yl)ethyl]-3-chloro-4,6-dihydroxybenzoate (three-letter code: VC4) (formula: C<sub>22</sub>H<sub>20</sub>ClNO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			28	22	1	1	4		
5	B	1	Total	C	Cl	N	O	0	0
			28	22	1	1	4		

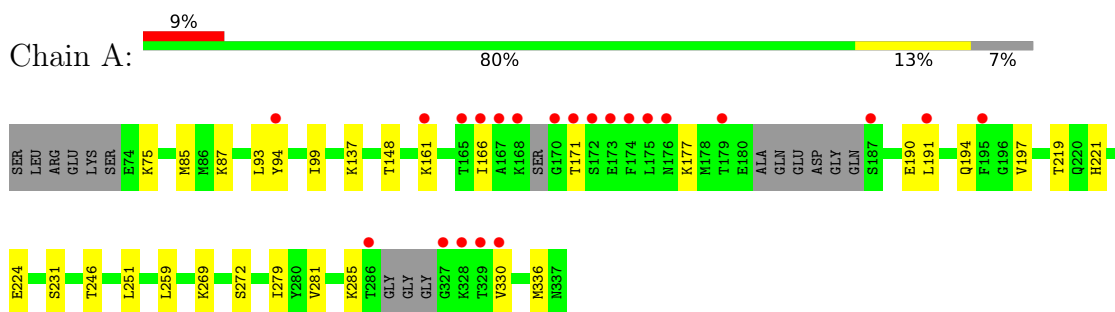
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	40	Total	O	0	0
			40	40		
6	B	38	Total	O	0	0
			38	38		

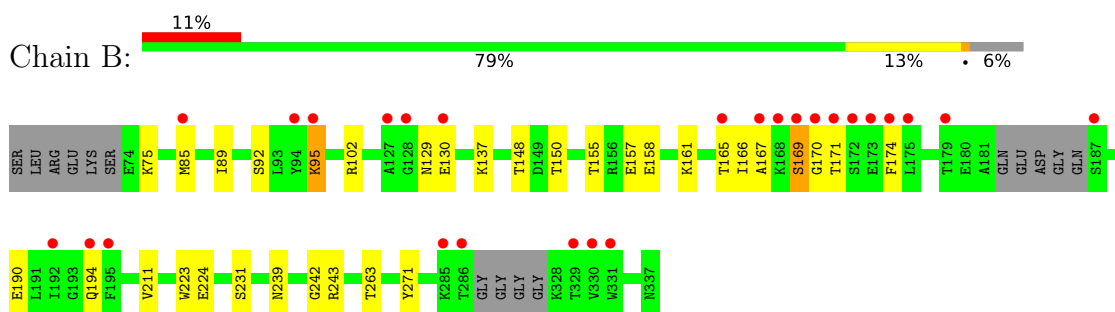
### 3 Residue-property plots [i](#)

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: Endoplasmic



- Molecule 1: Endoplasmic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.43Å 84.72Å 95.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.36 – 2.35 42.36 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.36-2.35) 99.7 (42.36-2.35)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.16 (at 2.34Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.197 , 0.237 0.197 , 0.237	Depositor DCC
$R_{free}$ test set	1997 reflections (8.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtrriage
Anisotropy	0.499	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3737	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2869e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PE8, PEG, GOL, VC4

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	0/1737	0.52	2/2339 (0.1%)
1	B	0.28	0/1753	0.50	0/2363
All	All	0.27	0/3490	0.51	2/4702 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	LYS	CB-CG-CD	6.44	128.35	111.60
1	A	161	LYS	CD-CE-NZ	6.07	125.67	111.70

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	1713	0	1720	19	0
1	B	1728	0	1729	29	0
2	A	79	0	98	7	0
2	B	38	0	42	4	0
3	A	14	0	20	1	0
3	B	7	0	10	0	0
4	A	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	12	0	16	0	0
5	A	28	0	0	0	0
5	B	28	0	0	1	0
6	A	40	0	0	0	0
6	B	38	0	0	1	0
All	All	3737	0	3651	50	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 7.

All (50) 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:B:95:LYS:HD3	1:B:95:LYS:H	1.43	0.82
1:B:92:SER:O	1:B:95:LYS:NZ	2.17	0.70
1:A:87:LYS:HE3	2:A:401:PE8:H111	1.75	0.68
1:A:272:SER:HB2	1:A:279:ILE:HD12	1.80	0.64
1:B:150:THR:HG22	2:B:404:PE8:H51	1.83	0.60
1:A:87:LYS:HG3	2:A:401:PE8:H82	1.83	0.60
1:B:75:LYS:HD3	1:B:231:SER:HB3	1.85	0.57
1:B:157:GLU:O	1:B:161:LYS:HG2	2.03	0.57
1:B:137:LYS:HZ2	2:B:401:PE8:H121	1.71	0.55
1:A:137:LYS:HD3	2:A:403:PE8:H141	1.89	0.54
1:B:85:MET:HE3	1:B:89:ILE:HG13	1.90	0.54
1:B:161:LYS:O	1:B:165:THR:HB	2.08	0.53
1:B:224:GLU:OE1	1:B:231:SER:OG	2.22	0.52
1:B:169:SER:C	1:B:171:THR:H	2.13	0.52
1:A:246:THR:HG21	2:A:404:PE8:H111	1.92	0.52
1:A:137:LYS:HD3	2:A:403:PE8:H121	1.92	0.52
3:A:407:PEG:H12	1:B:263:THR:HG23	1.93	0.49
1:A:166:ILE:HG21	1:A:171:THR:HG21	1.95	0.49
1:B:239:ASN:HD21	1:B:242:GLY:H	1.60	0.49
1:B:239:ASN:ND2	1:B:242:GLY:H	2.11	0.48
1:A:219:THR:O	1:A:221:HIS:HD2	1.97	0.48
1:A:85:MET:HE3	1:A:197:VAL:HG11	1.96	0.48
1:A:177:LYS:HG3	1:A:191:LEU:HD11	1.97	0.47
1:A:251:LEU:HD12	1:A:259:LEU:HG	1.97	0.47
1:B:170:GLY:O	1:B:174:PHE:N	2.43	0.46
1:B:102:ARG:HB2	1:B:271:TYR:CG	2.50	0.46
1:B:169:SER:O	1:B:171:THR:N	2.48	0.46
1:B:129:ASN:O	1:B:243:ARG:NH1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HD23	1:A:99:ILE:HD11	1.98	0.45
1:A:285:LYS:HB2	1:A:330:VAL:HG13	1.97	0.45
1:B:85:MET:CE	1:B:89:ILE:HG13	2.47	0.45
1:B:137:LYS:HZ3	2:B:401:PE8:H91	1.82	0.45
1:B:166:ILE:CG2	1:B:171:THR:HG21	2.47	0.45
1:B:190:GLU:O	1:B:194:GLN:HG3	2.17	0.44
1:A:75:LYS:HD3	1:A:231:SER:HB3	1.99	0.44
1:B:165:THR:HG22	1:B:166:ILE:N	2.32	0.44
1:A:190:GLU:O	1:A:194:GLN:HG3	2.17	0.44
1:A:281:VAL:HG23	1:A:336:MET:HG3	1.99	0.43
1:B:211:VAL:HB	1:B:223:TRP:HB3	2.00	0.43
1:A:269:LYS:HD2	1:A:336:MET:O	2.18	0.43
1:B:148:THR:HG21	2:B:404:PE8:H81	2.00	0.43
4:A:411:GOL:O3	4:A:411:GOL:O1	2.36	0.42
1:B:155:THR:OG1	1:B:158:GLU:HG3	2.20	0.42
1:B:166:ILE:HG23	1:B:171:THR:HG21	2.00	0.42
1:B:166:ILE:HG13	1:B:167:ALA:H	1.84	0.42
1:A:148:THR:HG21	2:A:405:PE8:H51	2.02	0.42
1:B:169:SER:O	1:B:171:THR:HG23	2.20	0.42
5:B:410:VC4:O05	6:B:501:HOH:O	2.21	0.41
1:A:87:LYS:HD3	2:A:401:PE8:H241	2.03	0.41
1:B:169:SER:C	1:B:171:THR:N	2.74	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	209/233 (90%)	201 (96%)	8 (4%)	0	<b>100</b> <b>100</b>
1	B	212/233 (91%)	203 (96%)	8 (4%)	1 (0%)	29 32
All	All	421/466 (90%)	404 (96%)	16 (4%)	1 (0%)	47 56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	169	SER

### 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	190/205 (93%)	188 (99%)	2 (1%)	73	84
1	B	193/205 (94%)	191 (99%)	2 (1%)	76	85
All	All	383/410 (93%)	379 (99%)	4 (1%)	76	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	TYR
1	A	224	GLU
1	B	95	LYS
1	B	130	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	221	HIS
1	B	146	HIS
1	B	176	ASN
1	B	239	ASN
1	B	266	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

22 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
2	PE8	A	406	-	3,3,24	0.59	0	2,2,23	0.87	0
2	PE8	B	405	-	3,3,24	0.60	0	2,2,23	0.91	0
3	PEG	A	408	-	6,6,6	0.68	0	5,5,5	0.79	0
5	VC4	A	412	-	30,30,30	1.66	2 (6%)	37,41,41	2.13	13 (35%)
2	PE8	A	402	-	12,12,24	0.72	0	11,11,23	0.72	0
2	PE8	A	404	-	12,12,24	0.72	0	11,11,23	0.77	0
3	PEG	B	407	-	6,6,6	0.67	0	5,5,5	0.90	0
2	PE8	A	403	-	15,15,24	0.72	0	14,14,23	0.67	0
4	GOL	B	408	-	5,5,5	0.87	0	5,5,5	0.92	0
2	PE8	A	401	-	24,24,24	0.70	0	23,23,23	0.78	0
3	PEG	A	407	-	6,6,6	0.68	0	5,5,5	0.78	0
4	GOL	B	409	-	5,5,5	0.85	0	5,5,5	0.90	0
5	VC4	B	410	-	30,30,30	1.57	3 (10%)	37,41,41	2.23	13 (35%)
2	PE8	B	402	-	3,3,24	0.60	0	2,2,23	0.89	0
2	PE8	B	401	-	15,15,24	0.72	0	14,14,23	0.66	0
2	PE8	B	403	-	3,3,24	0.59	0	2,2,23	0.86	0
4	GOL	A	411	-	5,5,5	0.77	0	5,5,5	1.12	0
2	PE8	B	404	-	5,5,24	0.72	0	4,4,23	0.73	0
4	GOL	A	410	-	5,5,5	0.86	0	5,5,5	0.94	0
2	PE8	B	406	-	3,3,24	0.60	0	2,2,23	0.87	0
2	PE8	A	405	-	3,3,24	0.59	0	2,2,23	0.86	0
2	PE8	A	409	-	3,3,24	0.59	0	2,2,23	0.85	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	PE8	A	406	-	-	1/1/1/22	-
2	PE8	B	405	-	-	0/1/1/22	-
3	PEG	A	408	-	-	3/4/4/4	-
5	VC4	A	412	-	-	5/15/15/15	0/3/3/3
2	PE8	A	402	-	-	7/10/10/22	-
2	PE8	A	404	-	-	5/10/10/22	-
3	PEG	B	407	-	-	2/4/4/4	-
2	PE8	A	403	-	-	6/13/13/22	-
4	GOL	B	408	-	-	2/4/4/4	-
2	PE8	A	401	-	-	10/22/22/22	-
3	PEG	A	407	-	-	4/4/4/4	-
4	GOL	B	409	-	-	2/4/4/4	-
5	VC4	B	410	-	-	4/15/15/15	0/3/3/3
2	PE8	B	402	-	-	1/1/1/22	-
2	PE8	B	401	-	-	6/13/13/22	-
2	PE8	B	403	-	-	1/1/1/22	-
4	GOL	A	411	-	-	0/4/4/4	-
2	PE8	B	404	-	-	0/3/3/22	-
4	GOL	A	410	-	-	2/4/4/4	-
2	PE8	B	406	-	-	0/1/1/22	-
2	PE8	A	405	-	-	1/1/1/22	-
2	PE8	A	409	-	-	0/1/1/22	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	412	VC4	C13-C12	7.18	1.57	1.51
5	B	410	VC4	C13-C12	6.36	1.56	1.51
5	B	410	VC4	C11-C12	2.11	1.45	1.41
5	A	412	VC4	C11-C12	2.11	1.45	1.41
5	B	410	VC4	C09-C08	2.10	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	410	VC4	C09-C10-C11	8.48	126.53	112.81
5	A	412	VC4	C09-C10-C11	7.67	125.22	112.81
5	B	410	VC4	O26-C25-O28	-3.65	116.31	123.45
5	A	412	VC4	O26-C25-O28	-3.63	116.36	123.45
5	B	410	VC4	O26-C25-C24	3.61	120.92	112.27
5	A	412	VC4	O26-C25-C24	3.50	120.67	112.27
5	B	410	VC4	C21-N20-C12	3.14	121.76	117.81
5	A	412	VC4	C21-N20-C12	3.10	121.71	117.81
5	B	410	VC4	C23-C11-C12	-2.91	115.40	117.33
5	A	412	VC4	C23-C11-C12	-2.82	115.47	117.33
5	B	410	VC4	C04-C06-CL7	-2.79	114.40	119.12
5	A	412	VC4	C11-C12-N20	-2.79	120.67	122.76
5	A	412	VC4	C10-C09-C08	2.74	117.55	112.49
5	B	410	VC4	C11-C12-N20	-2.73	120.71	122.76
5	B	410	VC4	C14-C13-C12	2.54	118.91	112.40
5	A	412	VC4	C14-C13-C12	2.49	118.78	112.40
5	A	412	VC4	C04-C06-CL7	-2.46	114.97	119.12
5	B	410	VC4	C10-C09-C08	2.38	116.88	112.49
5	B	410	VC4	C03-C02-C24	2.29	123.59	120.93
5	A	412	VC4	C04-C03-C02	-2.27	117.88	120.14
5	B	410	VC4	C09-C08-C24	2.27	124.82	120.65
5	B	410	VC4	C04-C03-C02	-2.26	117.89	120.14
5	A	412	VC4	C03-C02-C24	2.17	123.46	120.93
5	A	412	VC4	C09-C08-C24	2.09	124.49	120.65
5	A	412	VC4	O01-C02-C24	-2.05	117.31	121.14
5	B	410	VC4	O01-C02-C24	-2.04	117.32	121.14

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	410	GOL	C1-C2-C3-O3
5	A	412	VC4	C11-C12-C13-C14
5	A	412	VC4	N20-C12-C13-C14
5	B	410	VC4	C11-C12-C13-C14
5	B	410	VC4	N20-C12-C13-C14
3	A	408	PEG	O2-C3-C4-O4
2	B	401	PE8	O13-C14-C15-O16
2	A	402	PE8	O7-C8-C9-O10
2	A	404	PE8	O7-C8-C9-O10
2	A	401	PE8	O13-C14-C15-O16
2	A	403	PE8	O10-C11-C12-O13
2	B	401	PE8	O7-C8-C9-O10

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Mol	Chain	Res	Type	Atoms
2	A	402	PE8	O4-C5-C6-O7
2	A	401	PE8	O19-C20-C21-O22
2	A	401	PE8	O7-C8-C9-O10
2	B	401	PE8	O10-C11-C12-O13
2	B	401	PE8	C12-C11-O10-C9
2	A	401	PE8	O4-C5-C6-O7
2	A	401	PE8	O1-C2-C3-O4
2	A	403	PE8	O16-C17-C18-O19
4	B	408	GOL	O1-C1-C2-C3
4	B	409	GOL	C1-C2-C3-O3
2	A	404	PE8	O13-C14-C15-O16
2	A	402	PE8	O10-C11-C12-O13
2	B	402	PE8	O4-C5-C6-O7
2	B	403	PE8	O4-C5-C6-O7
2	A	402	PE8	O13-C14-C15-O16
2	A	403	PE8	O4-C5-C6-O7
2	B	401	PE8	O4-C5-C6-O7
3	A	408	PEG	O1-C1-C2-O2
2	A	403	PE8	O13-C14-C15-O16
4	A	410	GOL	O2-C2-C3-O3
2	A	404	PE8	O10-C11-C12-O13
3	A	407	PEG	O2-C3-C4-O4
5	A	412	VC4	C08-C09-C10-C11
2	A	405	PE8	O4-C5-C6-O7
2	A	406	PE8	O4-C5-C6-O7
3	B	407	PEG	O2-C3-C4-O4
2	A	402	PE8	C12-C11-O10-C9
2	A	402	PE8	C11-C12-O13-C14
2	A	404	PE8	C11-C12-O13-C14
3	A	407	PEG	C1-C2-O2-C3
4	B	408	GOL	O1-C1-C2-O2
2	A	401	PE8	O10-C11-C12-O13
2	A	403	PE8	C11-C12-O13-C14
2	A	402	PE8	C9-C8-O7-C6
2	A	404	PE8	C9-C8-O7-C6
3	A	407	PEG	O1-C1-C2-O2
2	A	401	PE8	C20-C21-O22-C23
3	B	407	PEG	C4-C3-O2-C2
2	A	401	PE8	C6-C5-O4-C3
2	A	401	PE8	O22-C23-C24-O25
3	A	408	PEG	C4-C3-O2-C2
4	B	409	GOL	O2-C2-C3-O3

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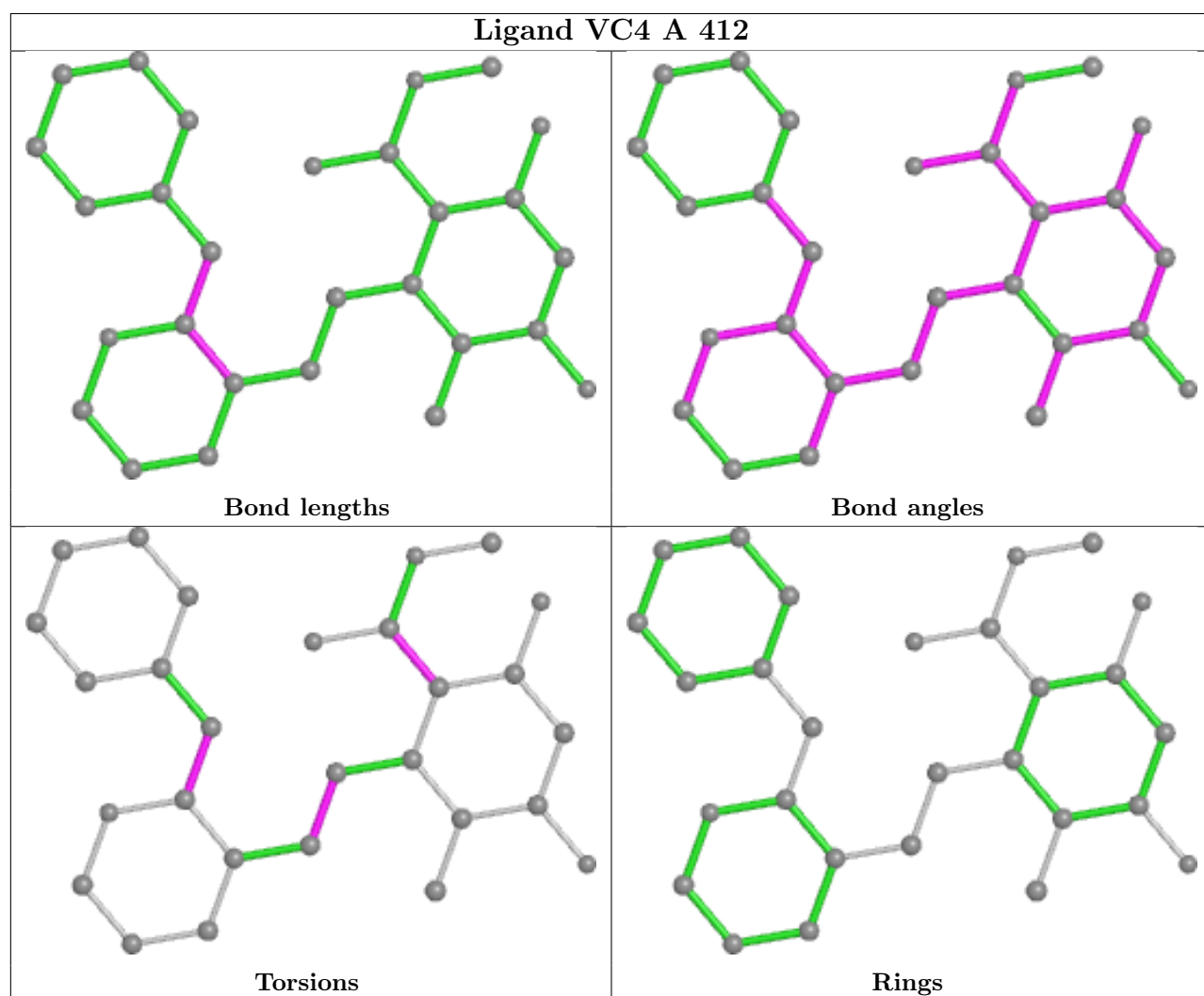
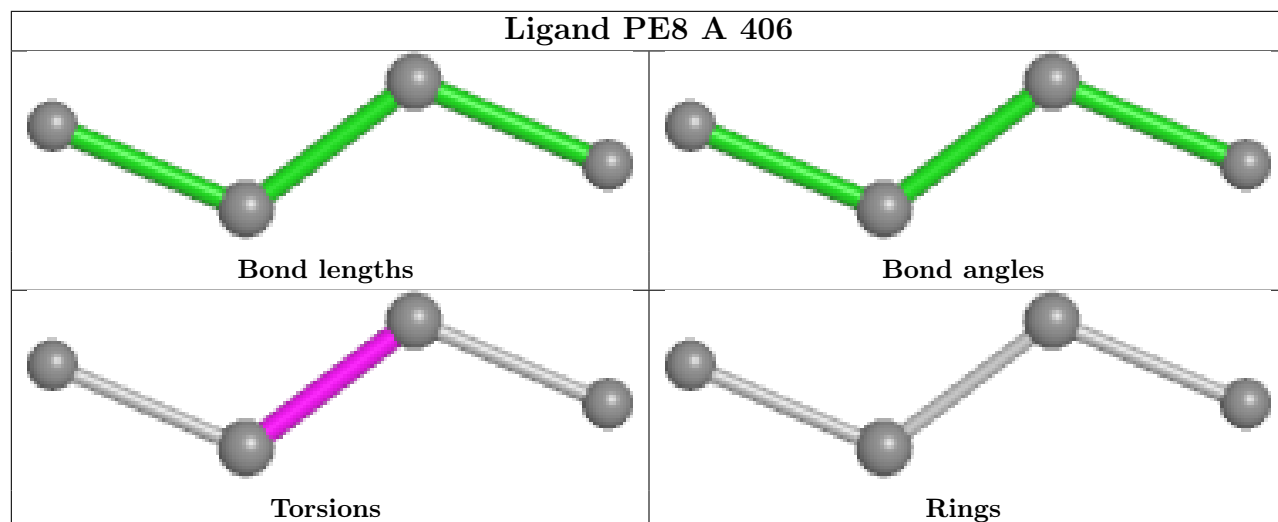
Mol	Chain	Res	Type	Atoms
2	A	401	PE8	C18-C17-O16-C15
5	A	412	VC4	C02-C24-C25-O26
5	A	412	VC4	C02-C24-C25-O28
2	A	403	PE8	C8-C9-O10-C11
5	B	410	VC4	C02-C24-C25-O26
5	B	410	VC4	C02-C24-C25-O28
3	A	407	PEG	C4-C3-O2-C2
2	B	401	PE8	C18-C17-O16-C15

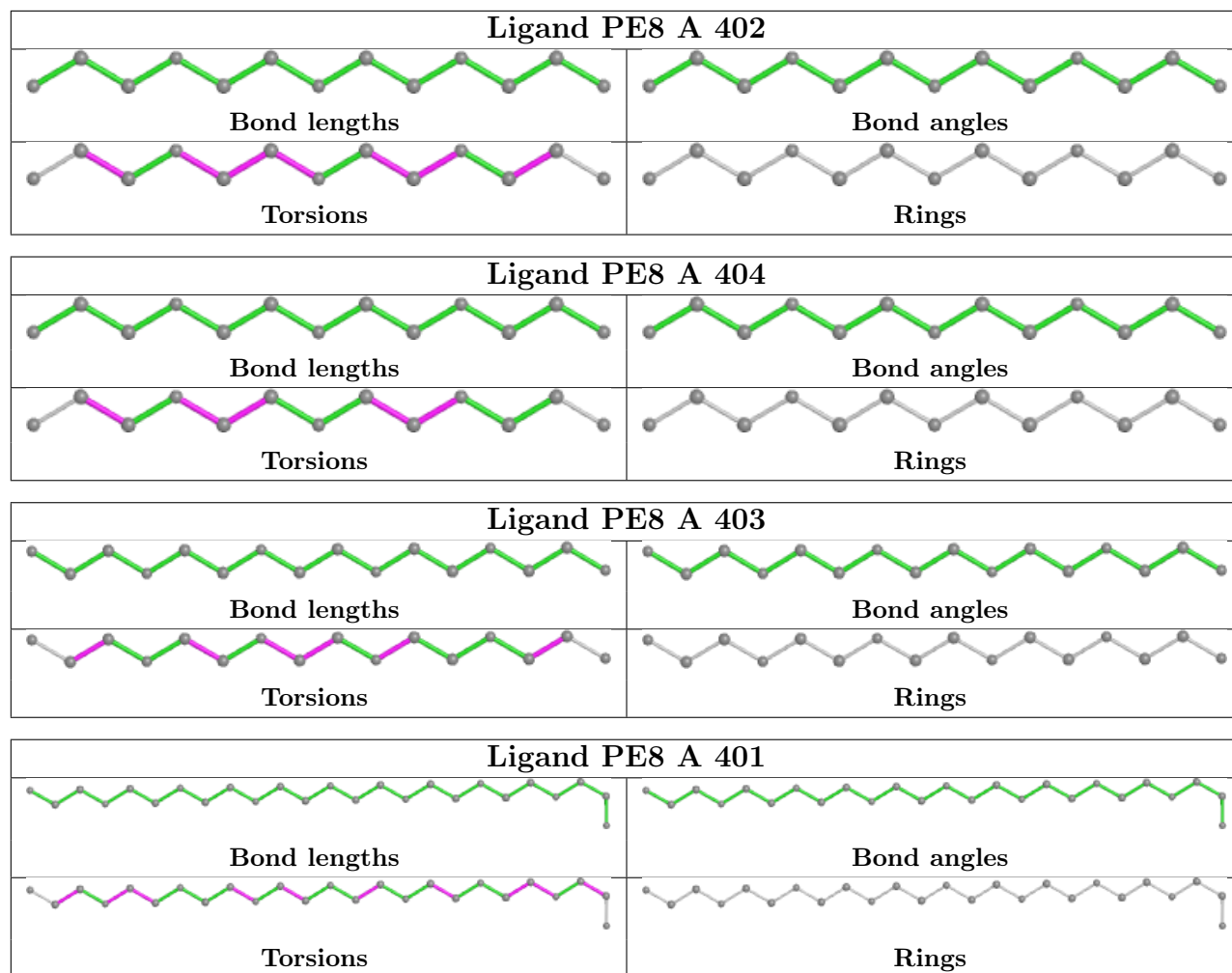
There are no ring outliers.

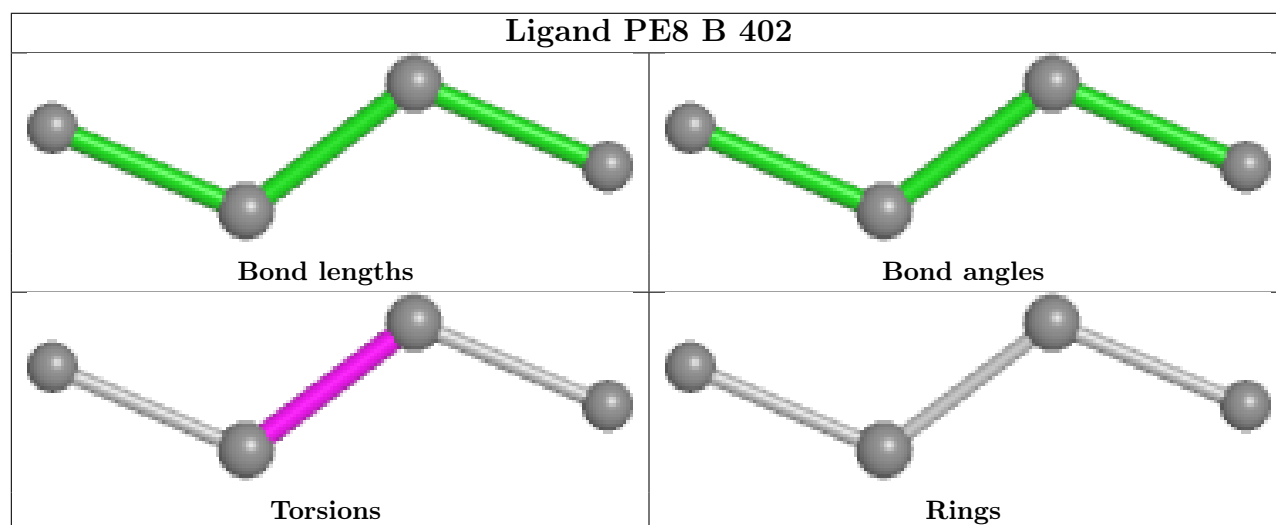
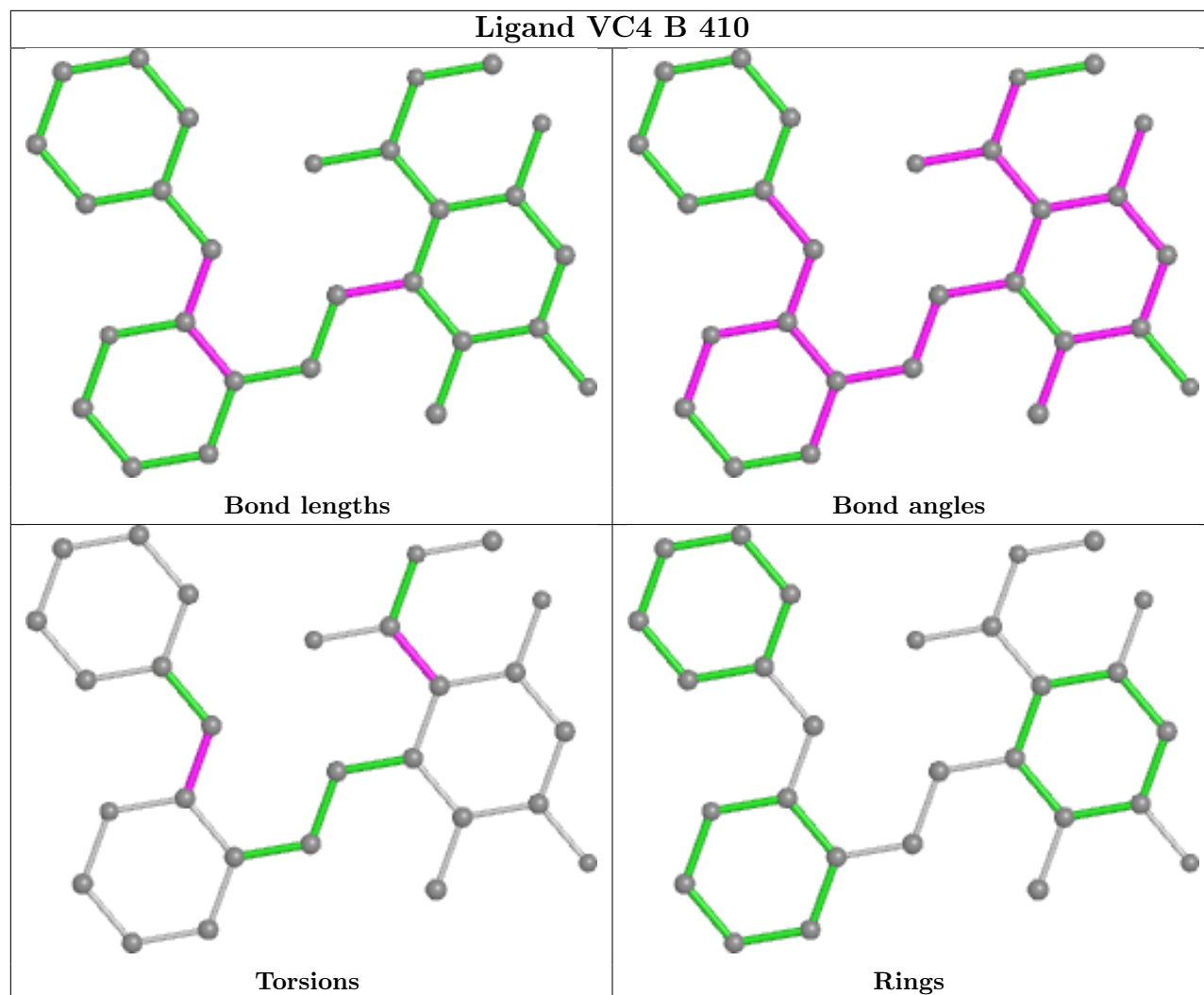
9 monomers are involved in 14 short contacts:

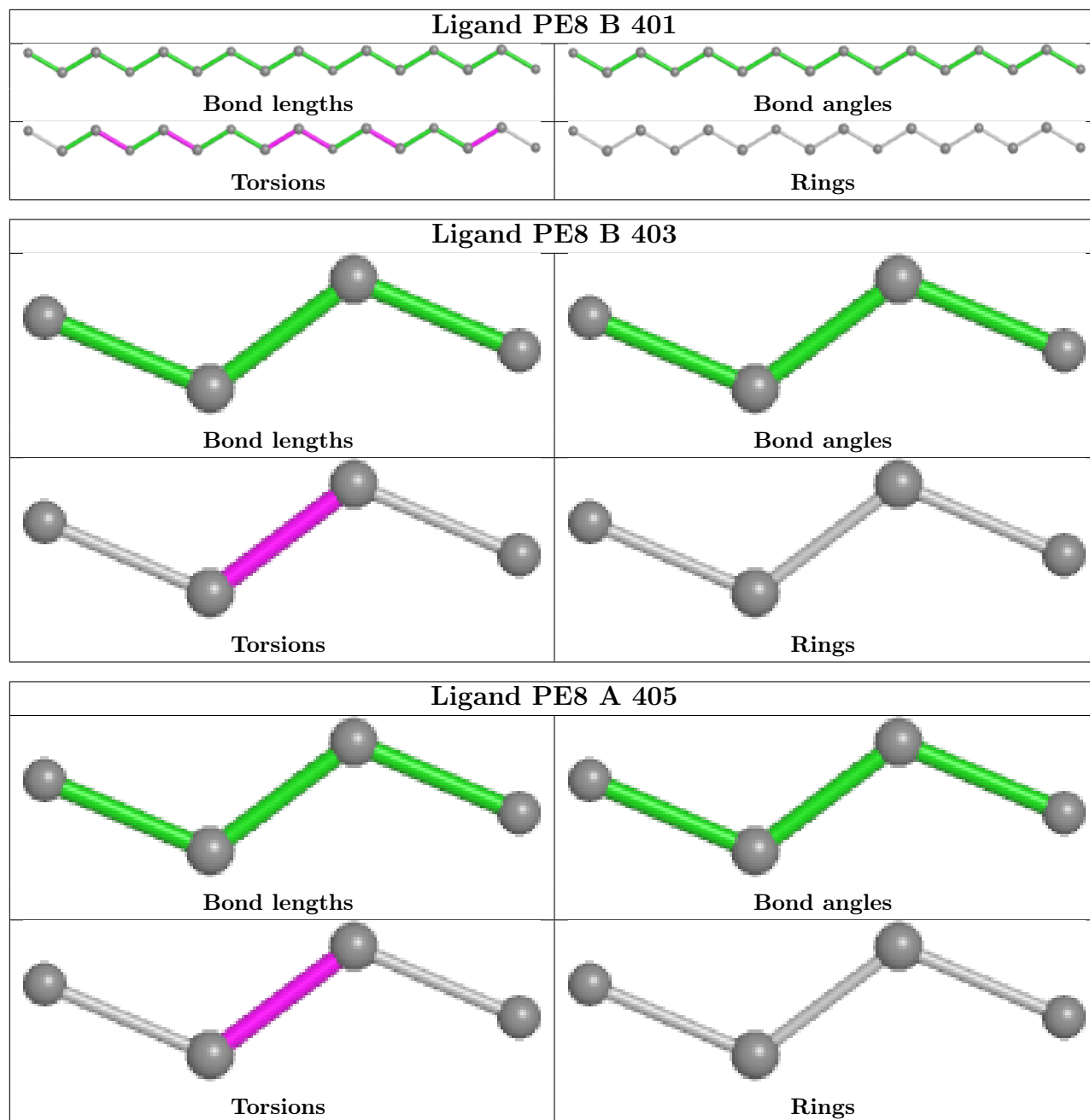
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	PE8	1	0
2	A	403	PE8	2	0
2	A	401	PE8	3	0
3	A	407	PEG	1	0
5	B	410	VC4	1	0
2	B	401	PE8	2	0
4	A	411	GOL	1	0
2	B	404	PE8	2	0
2	A	405	PE8	1	0

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

### 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, 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	217/233 (93%)	0.39	22 (10%) <b>7</b> <b>11</b>	20, 36, 95, 127	0
1	B	218/233 (93%)	0.47	26 (11%) <b>4</b> <b>7</b>	19, 35, 92, 123	0
All	All	435/466 (93%)	0.43	48 (11%) <b>5</b> <b>8</b>	19, 36, 94, 127	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	LYS	7.8
1	B	169	SER	7.0
1	A	173	GLU	6.0
1	B	167	ALA	6.0
1	A	167	ALA	5.9
1	B	170	GLY	5.7
1	B	173	GLU	5.7
1	A	171	THR	5.0
1	A	328	LYS	4.8
1	A	172	SER	4.7
1	A	176	ASN	4.2
1	A	175	LEU	4.0
1	B	329	THR	4.0
1	B	168	LYS	3.9
1	B	127	ALA	3.9
1	A	170	GLY	3.8
1	A	329	THR	3.8
1	B	174	PHE	3.6
1	B	330	VAL	3.6
1	B	171	THR	3.5
1	B	187	SER	3.5
1	B	175	LEU	3.4
1	A	330	VAL	3.3
1	A	191	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	286	THR	3.1
1	B	179	THR	3.0
1	A	165	THR	2.9
1	A	286	THR	2.8
1	A	187	SER	2.8
1	A	179	THR	2.8
1	A	94	TYR	2.7
1	A	174	PHE	2.6
1	B	172	SER	2.5
1	A	327	GLY	2.5
1	B	94	TYR	2.4
1	B	195	PHE	2.4
1	B	85	MET	2.3
1	B	331	TRP	2.3
1	B	128	GLY	2.3
1	A	166	ILE	2.3
1	B	165	THR	2.3
1	B	95	LYS	2.3
1	A	161	LYS	2.2
1	A	195	PHE	2.2
1	B	285	LYS	2.1
1	B	194	GLN	2.1
1	B	192	ILE	2.1
1	B	130	GLU	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.

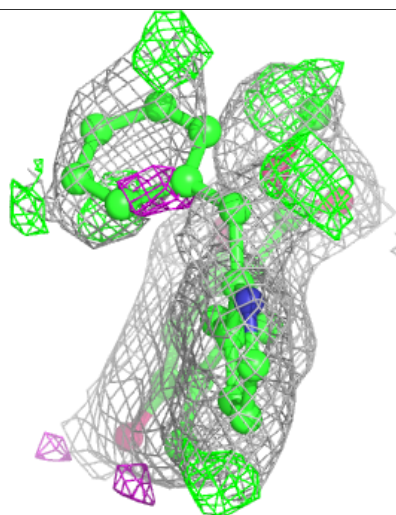
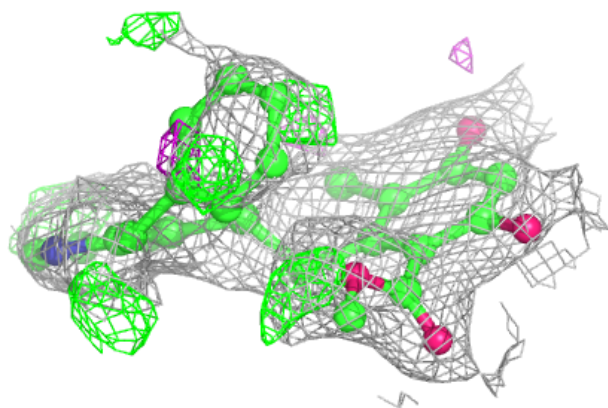
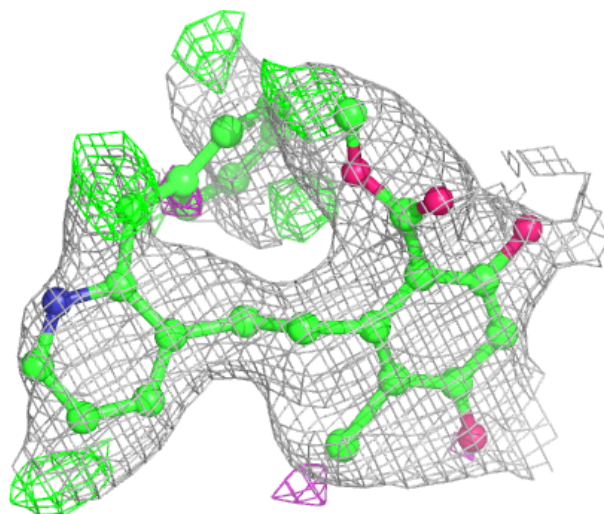
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	B	408	6/6	0.79	0.22	67,70,70,71	0
5	VC4	B	410	28/28	0.79	0.24	40,61,89,91	0
3	PEG	B	407	7/7	0.80	0.36	76,77,86,89	0
2	PE8	A	403	16/25	0.81	0.20	59,65,70,70	0
5	VC4	A	412	28/28	0.82	0.26	45,63,78,80	0
2	PE8	B	403	4/25	0.82	0.21	54,55,59,61	0
3	PEG	A	408	7/7	0.83	0.21	65,67,69,70	0
2	PE8	A	409	4/25	0.84	0.20	67,71,72,73	0
2	PE8	B	402	4/25	0.84	0.16	60,63,63,64	0
2	PE8	A	405	4/25	0.85	0.34	53,57,57,57	0
2	PE8	B	404	6/25	0.87	0.47	46,47,48,48	0
2	PE8	B	405	4/25	0.87	0.26	66,68,69,70	0
4	GOL	A	410	6/6	0.87	0.23	68,72,74,74	0
2	PE8	A	406	4/25	0.88	0.19	58,59,62,67	0
2	PE8	A	401	25/25	0.88	0.20	32,44,68,70	0
4	GOL	A	411	6/6	0.89	0.20	72,74,75,75	0
2	PE8	B	401	16/25	0.90	0.18	47,59,65,68	0
2	PE8	B	406	4/25	0.90	0.18	59,61,61,64	0
2	PE8	A	402	13/25	0.90	0.19	48,53,60,63	0
2	PE8	A	404	13/25	0.91	0.17	48,53,61,63	0
4	GOL	B	409	6/6	0.91	0.22	63,66,69,72	0
3	PEG	A	407	7/7	0.92	0.23	58,59,71,74	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.



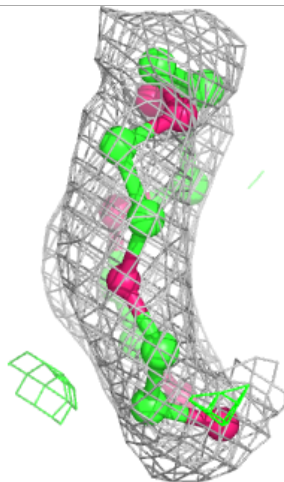
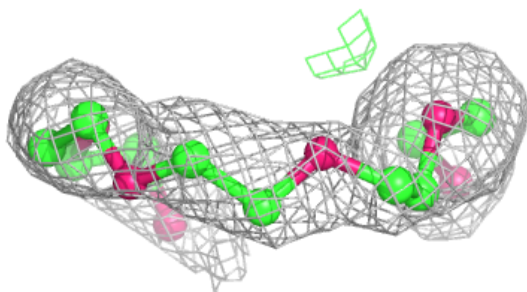
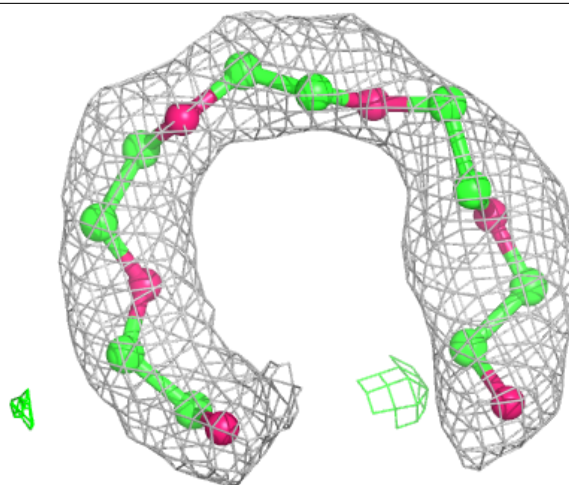
**Electron density around VC4 B 410:**

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



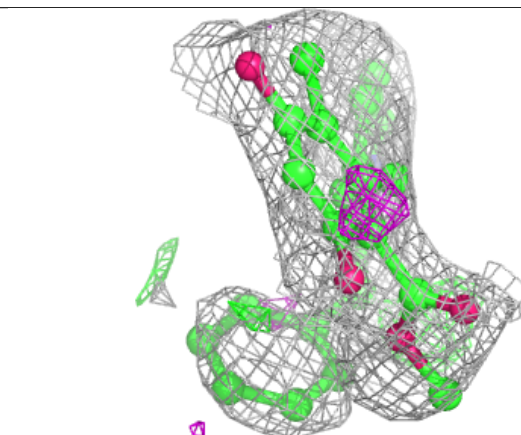
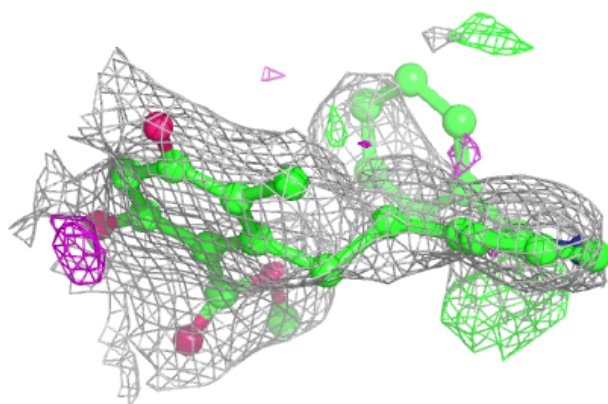
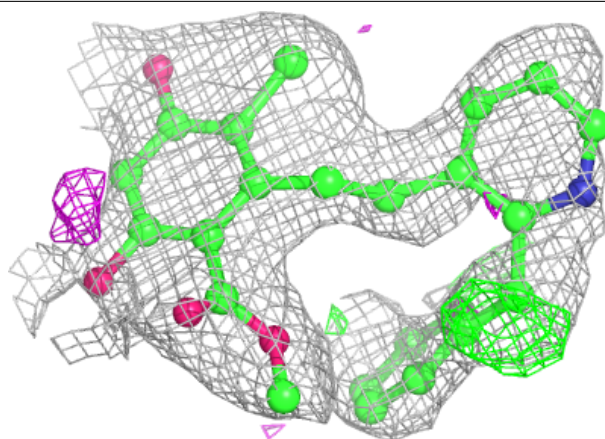
**Electron density around PE8 A 403:**

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

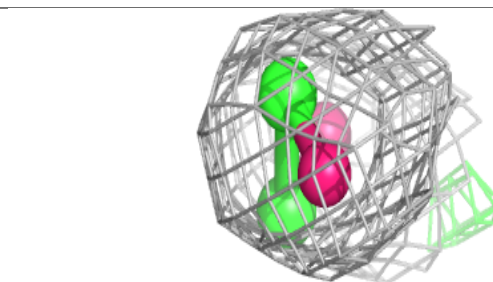
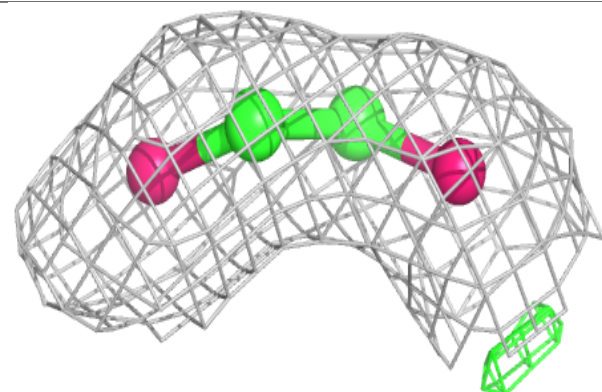
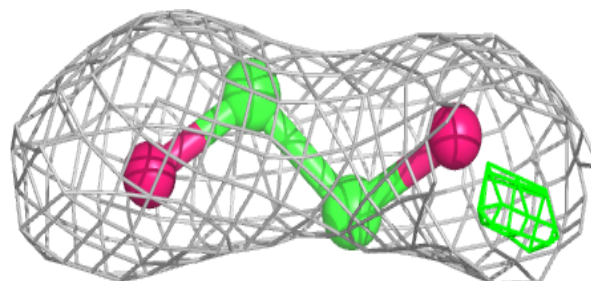


**Electron density around VC4 A 412:**

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

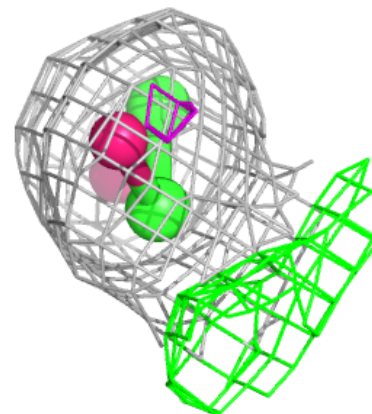
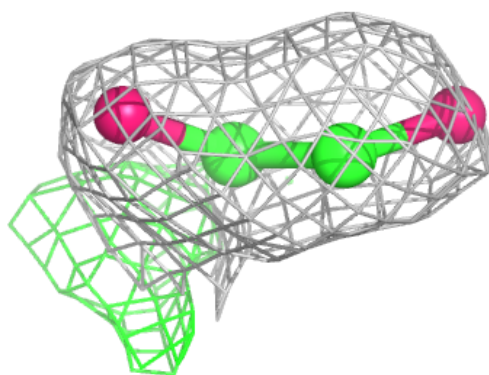
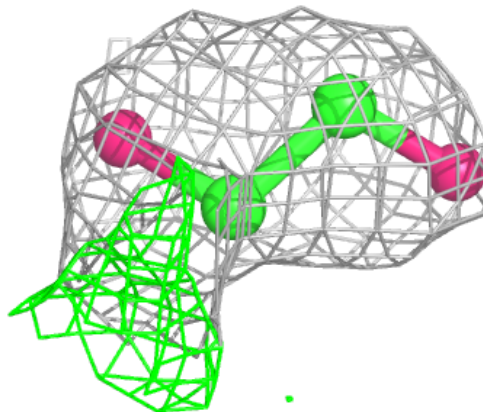
**Electron density around PE8 B 403:**

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



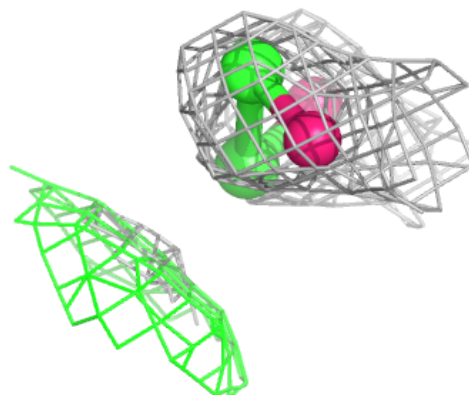
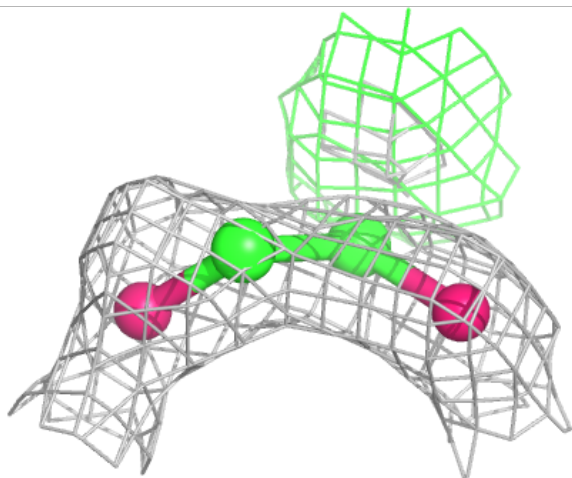
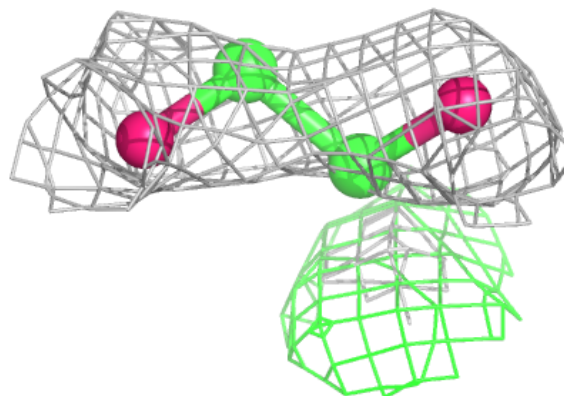
**Electron density around PE8 B 402:**

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



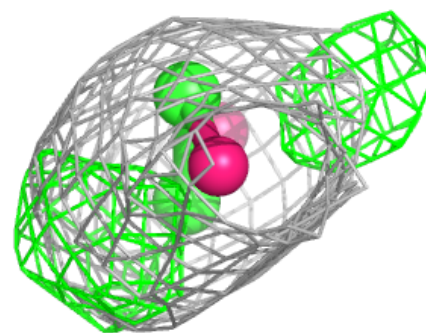
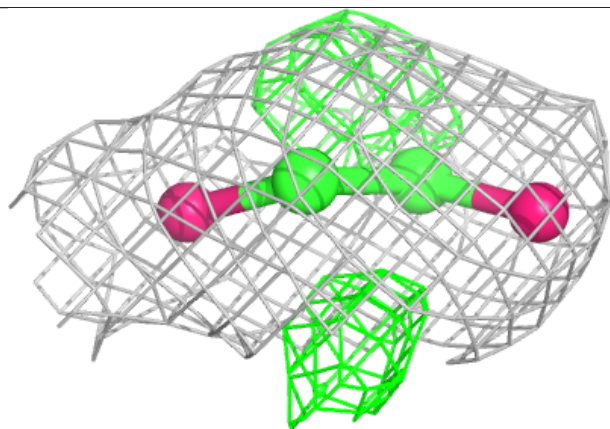
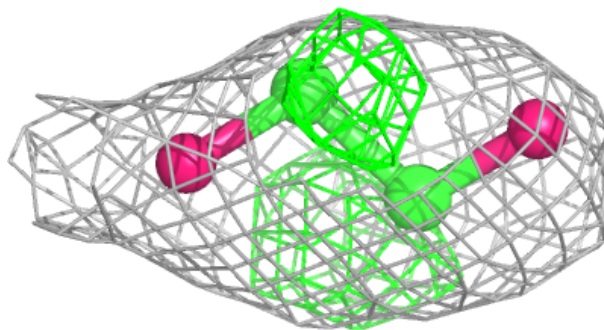
**Electron density around PE8 A 405:**

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and green (positive)

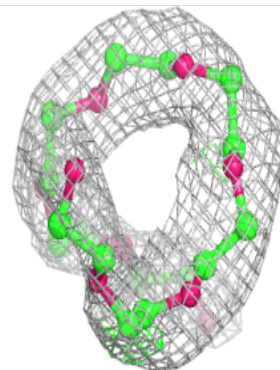
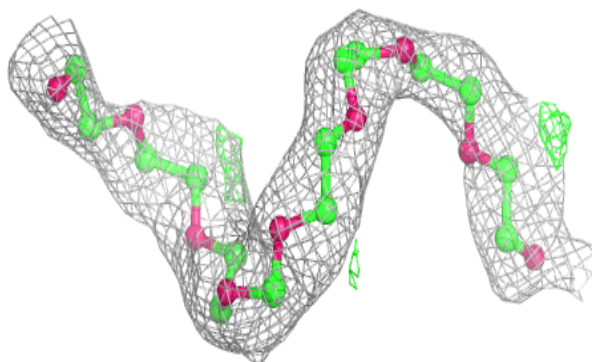
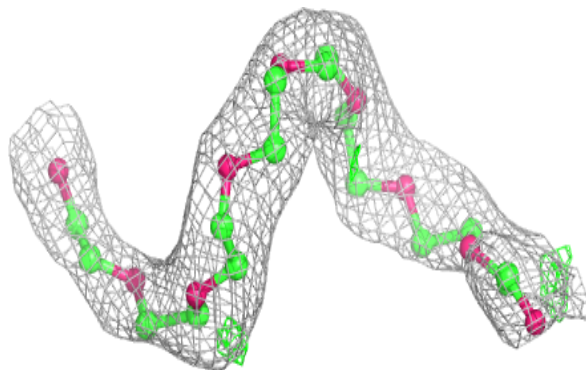


**Electron density around PE8 A 406:**

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

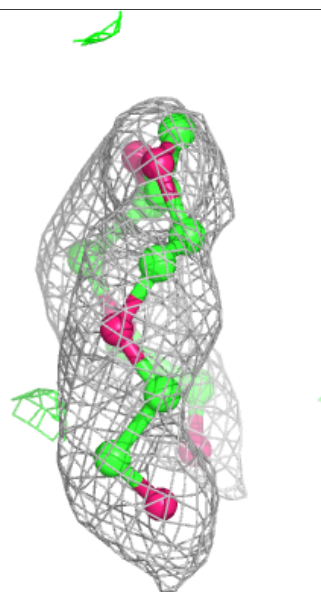
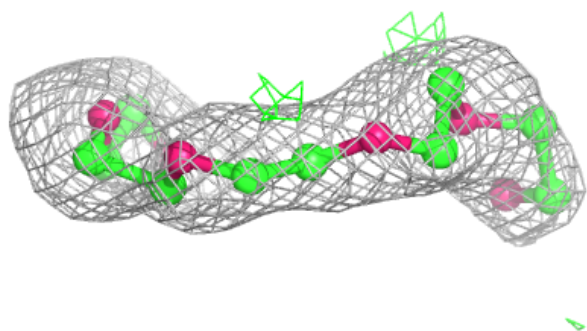
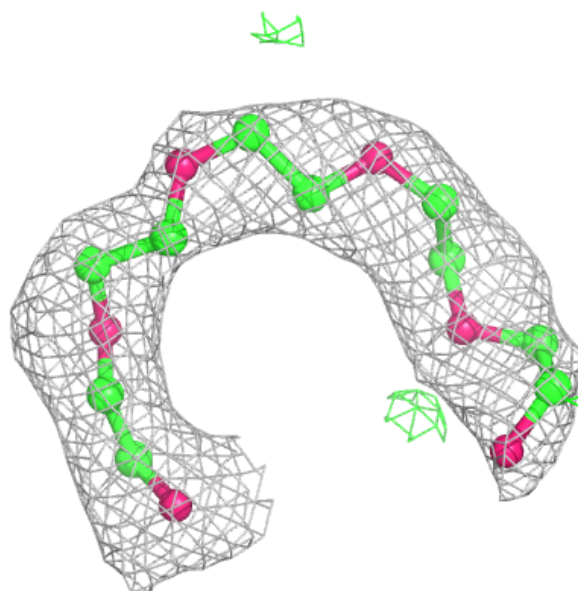
**Electron density around PE8 A 401:**

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



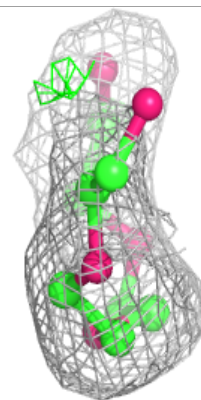
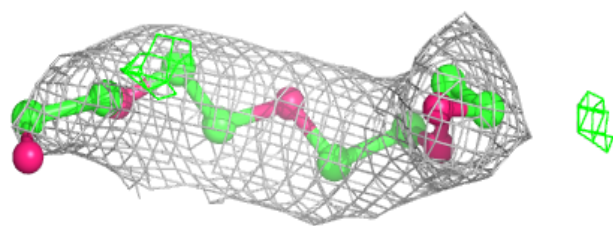
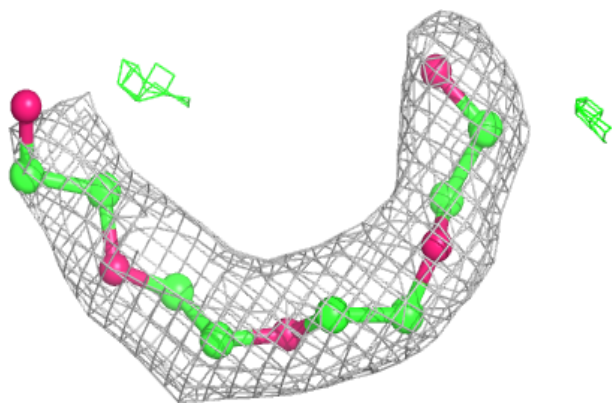
**Electron density around PE8 B 401:**

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

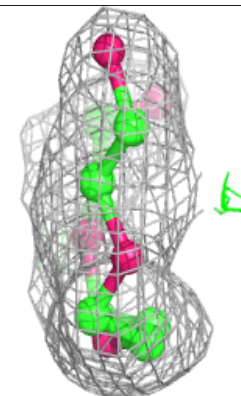
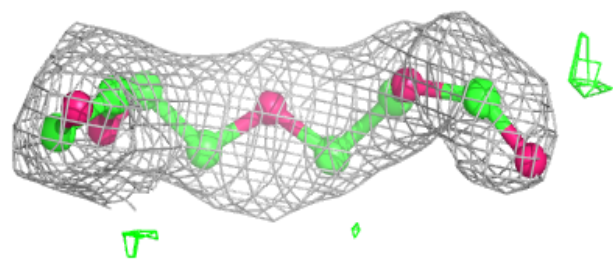
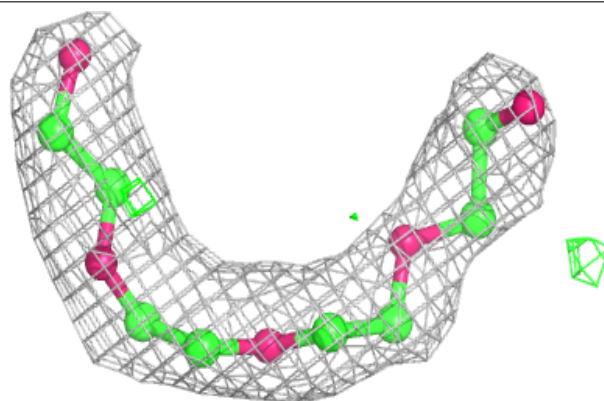


**Electron density around PE8 A 402:**

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

**Electron density around PE8 A 404:**

$2mF_o-DF_c$  (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.