



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 09:37 am GMT

PDB ID : 4BTL  
Title : Aromatic interactions in acetylcholinesterase-inhibitor complexes  
Authors : Andersson, C.D.; Forsgren, N.; Akfur, C.; Allgardsson, A.; Qian, W.; Engdahl, C.; Berg, L.; Ekstrom, F.; Linusson, A.  
Deposited on : 2013-06-18  
Resolution : 2.50 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

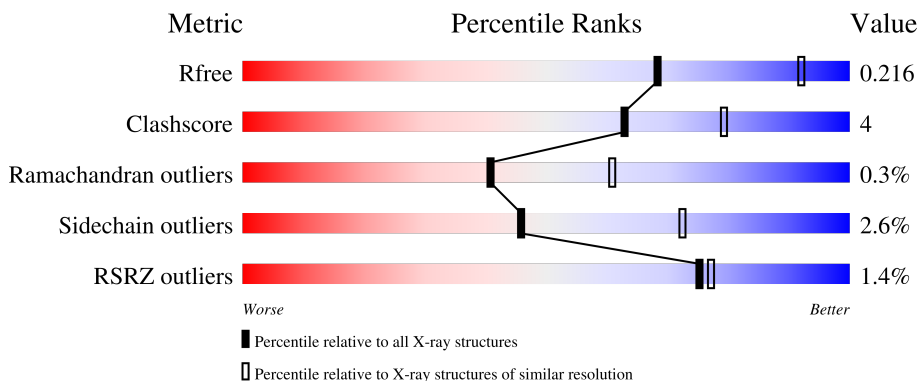
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


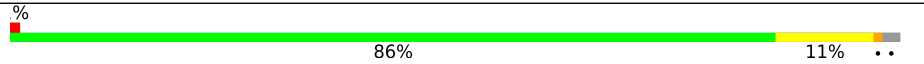
The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	543	
1	B	543	

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
3	NAG	A	1544	X	-	-	X
3	NAG	B	1546	X	-	-	-
3	NAG	B	1548	X	-	-	-

## 2 Entry composition [i](#)

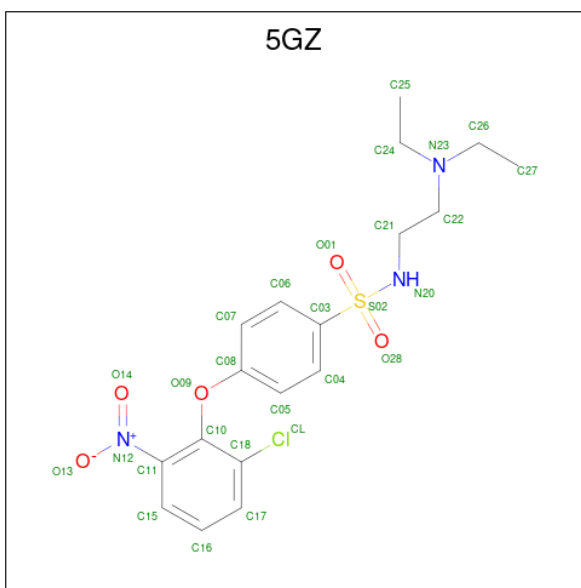
There are 6 unique types of molecules in this entry. The entry contains 8961 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	535	Total	C	N	O	S	0	4	0
			4209	2698	734	763	14			
1	B	534	Total	C	N	O	S	0	2	0
			4171	2677	723	757	14			

- Molecule 2 is 4-(2-chloro-6-nitrophenoxy)-N-[2-(diethylamino)ethyl]benzenesulfonamide (three-letter code: 5GZ) (formula: C<sub>18</sub>H<sub>22</sub>ClN<sub>3</sub>O<sub>5</sub>S).



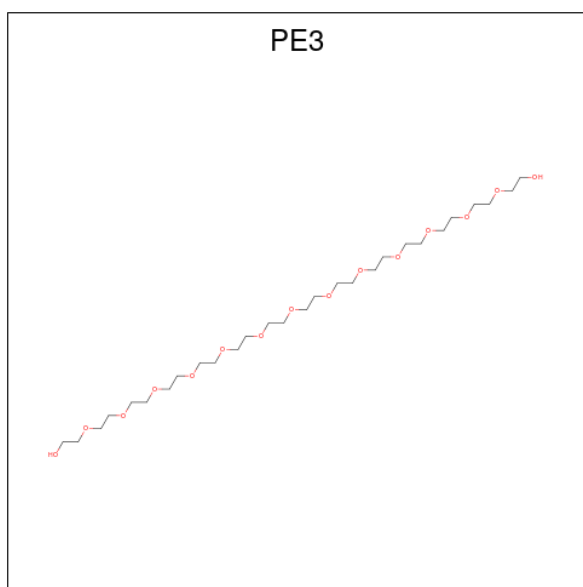
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
2	A	1	Total	C	Cl	N	O	S	0	0
			28	18	1	3	5	1		
2	A	1	Total	C	Cl	N	O	S	0	0
			22	13	1	2	5	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			28	18	1	3	5	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			23	14	1	2	5	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAXAHENTETRACONTANE-1,41-DIOL (three-letter code: PE3) (formula:  $C_{28}H_{58}O_{15}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			22	14	8		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

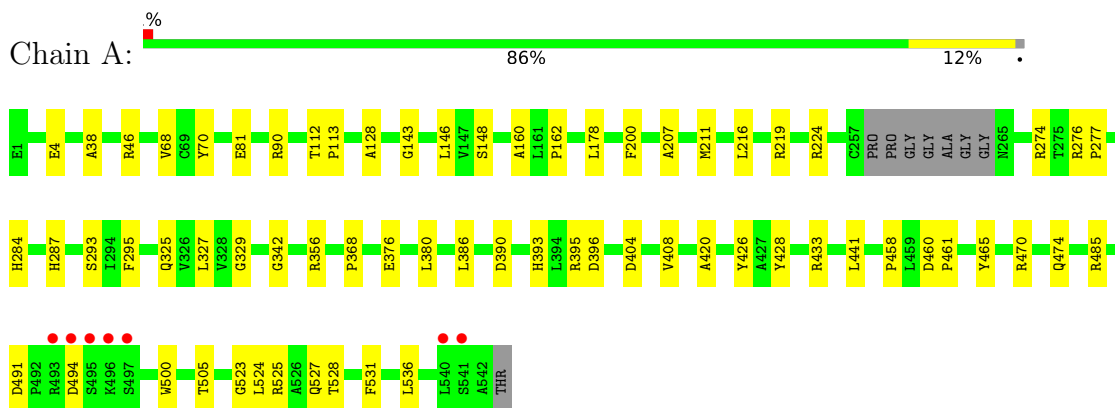
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	169	Total O 169 169	0	0
6	B	149	Total O 149 149	0	0

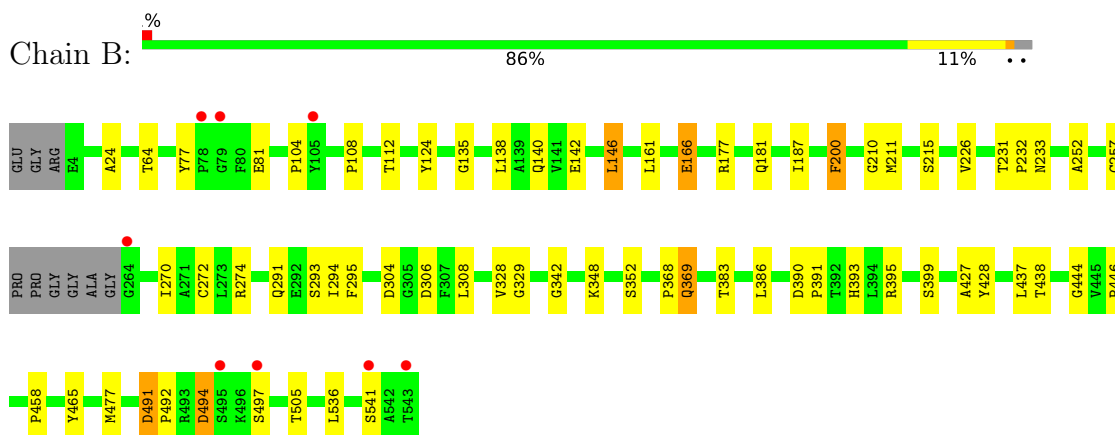
### 3 Residue-property plots [i](#)

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: ACETYLCHOLINESTERASE



#### • Molecule 1: ACETYLCHOLINESTERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.67Å 110.82Å 227.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.81 – 2.50 28.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (28.81-2.50) 99.5 (28.95-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.191 , 0.232 0.181 , 0.216	Depositor DCC
$R_{free}$ test set	1391 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.3	Xtrriage
Anisotropy	0.918	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8961	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5GZ, NAG, EDO, PE3

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	0.37	0/4336	0.55	0/5923
1	B	0.35	0/4297	0.53	0/5873
All	All	0.36	0/8633	0.54	0/11796

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

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	4209	0	4090	35	0
1	B	4171	0	4053	38	0
2	A	50	0	30	1	0
2	B	51	0	32	2	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
4	A	33	0	41	1	0
4	B	57	0	74	2	0
5	A	8	0	12	0	0
5	B	8	0	12	2	0
6	A	169	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	149	0	0	1	0
All	All	8961	0	8396	73	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 4.

All (73) 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)
4:A:1546:PE3:H391	2:A:1549:5GZ:H16	1.69	0.75
1:B:491:ASP:HB3	1:B:494:ASP:HB3	1.75	0.68
1:A:68:VAL:HG23	1:A:90[B]:ARG:HB2	1.84	0.60
4:B:1545:PE3:H382	2:B:1552:5GZ:H16	1.83	0.59
1:B:291:GLN:OE1	1:B:369[B]:GLN:NE2	2.36	0.59
1:B:252:ALA:HB1	1:B:257:CYS:HB2	1.86	0.58
1:B:294:ILE:HA	2:B:1544:5GZ:O14	2.06	0.55
1:A:46:ARG:O	1:A:274[B]:ARG:NH1	2.39	0.54
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.91	0.52
1:A:207:ALA:O	1:A:211:MET:HG2	2.09	0.52
1:A:395:ARG:HD2	1:A:396:ASP:OD1	2.09	0.52
1:A:458:PRO:HA	1:A:465:TYR:CD1	2.46	0.51
1:A:81:GLU:H	1:A:81:GLU:CD	2.14	0.51
1:A:527:GLN:NE2	1:B:383:THR:O	2.38	0.51
1:A:284:HIS:HA	1:A:287:HIS:HD2	1.76	0.50
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.94	0.50
1:A:327:LEU:HD11	1:A:500:TRP:CH2	2.46	0.50
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.47	0.49
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.94	0.49
1:A:376:GLU:O	1:A:380:LEU:HG	2.13	0.49
1:B:81:GLU:HG3	1:B:438:THR:HG21	1.95	0.48
1:A:404:ASP:OD1	1:A:525:ARG:NH1	2.46	0.48
1:B:177:ARG:NH2	1:B:215:SER:OG	2.44	0.48
1:A:420:ALA:HB2	1:A:505:THR:HG21	1.96	0.48
1:B:491:ASP:HA	1:B:492:PRO:HD3	1.76	0.47
1:A:523:GLY:HA3	1:B:386:LEU:HD21	1.96	0.47
1:A:527:GLN:HG3	4:B:1555:PE3:H261	1.96	0.47
1:A:390:ASP:HB3	1:A:393[B]:HIS:HB2	1.97	0.47
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.50	0.47
1:B:135:GLY:HA3	1:B:146:LEU:HD22	1.97	0.46
1:A:284:HIS:HA	1:A:287:HIS:CD2	2.49	0.46
1:A:219:ARG:HA	1:A:219:ARG:HD2	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:GLU:O	5:B:1549:EDO:H22	2.16	0.46
1:A:408:VAL:HG11	1:A:525:ARG:HG3	1.98	0.46
1:A:327:LEU:HD12	1:A:426:TYR:HB2	1.97	0.46
1:B:536:LEU:HD23	1:B:536:LEU:HA	1.79	0.45
1:A:528:THR:O	1:A:531:PHE:HB3	2.17	0.45
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.66	0.45
1:B:124:TYR:HB3	6:B:2060:HOH:O	2.17	0.45
1:B:231:THR:HB	1:B:233:ASN:OD1	2.17	0.44
1:B:328:VAL:O	1:B:427:ALA:HA	2.18	0.44
1:B:138:LEU:HD23	1:B:477:MET:HE3	2.00	0.44
1:B:112:THR:HG23	5:B:1549:EDO:H21	2.00	0.44
1:B:210:GLY:HA3	1:B:232:PRO:HD3	2.00	0.43
1:B:304:ASP:OD2	1:B:306:ASP:HB3	2.19	0.43
1:B:444:GLY:O	1:B:446:PRO:HD3	2.19	0.43
1:B:187:ILE:HD12	1:B:187:ILE:HA	1.89	0.43
1:B:390:ASP:HA	1:B:391:PRO:HD2	1.71	0.43
1:A:112:THR:HG21	1:A:143:GLY:O	2.19	0.43
1:B:166:GLU:HB2	1:B:274[A]:ARG:NH2	2.34	0.43
1:B:77:TYR:CD1	1:B:348:LYS:HE3	2.54	0.43
1:A:293:SER:HB3	1:A:368:PRO:HG3	2.01	0.42
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.82	0.42
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.55	0.42
1:A:160:ALA:O	1:A:162:PRO:HD3	2.20	0.42
1:A:460:ASP:HA	1:A:461:PRO:HD3	1.89	0.42
1:B:211:MET:HG2	1:B:308:LEU:HD21	2.01	0.42
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.55	0.42
1:A:128:ALA:HB1	1:A:148:SER:OG	2.20	0.42
1:A:470:ARG:O	1:A:474:GLN:HG3	2.19	0.42
1:A:491:ASP:HB3	1:A:494:ASP:HB3	2.01	0.41
1:B:166:GLU:HB2	1:B:274[A]:ARG:HH22	1.84	0.41
1:B:390:ASP:OD2	1:B:393:HIS:ND1	2.49	0.41
1:B:200:PHE:CB	1:B:226:VAL:HB	2.50	0.41
1:B:293:SER:HB3	1:B:368:PRO:HB3	2.01	0.41
1:A:224:ARG:HG2	1:A:325:GLN:HB2	2.02	0.41
1:A:433:ARG:NH2	1:A:441:LEU:HD23	2.35	0.41
1:B:104:PRO:HG2	1:B:108:PRO:HG3	2.01	0.41
1:B:211:MET:HG3	1:B:232:PRO:HB3	2.03	0.41
1:A:38:ALA:HB2	1:A:178:LEU:HD23	2.02	0.41
1:A:276:ARG:HA	1:A:277:PRO:HD3	1.99	0.40
1:B:352:SER:O	1:B:395:ARG:HG3	2.21	0.40
1:A:390:ASP:OD2	1:A:393[B]:HIS:ND1	2.49	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	535/543 (98%)	517 (97%)	17 (3%)	1 (0%)	47 68
1	B	532/543 (98%)	509 (96%)	21 (4%)	2 (0%)	34 54
All	All	1067/1086 (98%)	1026 (96%)	38 (4%)	3 (0%)	41 61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	497	SER
1	A	342	GLY
1	B	342	GLY

### 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	442/443 (100%)	433 (98%)	9 (2%)	55 79
1	B	438/443 (99%)	423 (97%)	15 (3%)	37 63
All	All	880/886 (99%)	856 (97%)	24 (3%)	46 71

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	70	TYR
1	A	146	LEU
1	A	200	PHE
1	A	216	LEU
1	A	295	PHE
1	A	356	ARG
1	A	386	LEU
1	A	524	LEU
1	B	64	THR
1	B	146	LEU
1	B	166	GLU
1	B	181	GLN
1	B	200	PHE
1	B	272	CYS
1	B	295	PHE
1	B	369[A]	GLN
1	B	369[B]	GLN
1	B	399	SER
1	B	437	LEU
1	B	491	ASP
1	B	494	ASP
1	B	505	THR
1	B	541	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

23 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
3	NAG	A	1544	1	14,14,15	0.50	0	17,19,21	1.00	2 (11%)
5	EDO	B	1549	-	3,3,3	0.64	0	2,2,2	0.84	0
4	PE3	B	1550	-	3,3,42	0.65	0	2,2,41	0.84	0
5	EDO	A	1548	-	3,3,3	0.71	0	2,2,2	0.76	0
4	PE3	A	1550	-	3,3,42	0.74	0	2,2,41	0.80	0
3	NAG	B	1548	1	14,14,15	0.71	0	17,19,21	1.92	5 (29%)
5	EDO	B	1554	-	3,3,3	0.65	0	2,2,2	0.93	0
4	PE3	B	1547	-	9,9,42	0.75	0	8,8,41	1.11	0
3	NAG	A	1547	1	14,14,15	0.48	0	17,19,21	1.21	1 (5%)
2	5GZ	A	1549	-	21,23,29	1.63	3 (14%)	28,33,40	2.20	8 (28%)
2	5GZ	B	1544	-	28,29,29	1.45	4 (14%)	36,40,40	1.97	7 (19%)
4	PE3	A	1545	-	4,4,42	0.41	0	3,3,41	1.04	0
4	PE3	A	1546	-	6,6,42	0.45	0	5,5,41	1.38	0
5	EDO	A	1551	-	3,3,3	0.62	0	2,2,2	0.91	0
4	PE3	A	1553	-	9,9,42	0.65	0	8,8,41	1.30	0
4	PE3	B	1545	-	6,6,42	0.54	0	5,5,41	1.33	0
4	PE3	B	1555	-	21,21,42	0.72	0	20,20,41	1.03	0
4	PE3	B	1553	-	6,6,42	0.32	0	5,5,41	1.53	0
2	5GZ	B	1552	-	23,24,29	1.70	2 (8%)	30,34,40	2.32	7 (23%)
4	PE3	A	1552	-	6,6,42	0.34	0	5,5,41	1.45	0
2	5GZ	A	1543	-	28,29,29	1.43	4 (14%)	36,40,40	1.85	6 (16%)
3	NAG	B	1546	1	14,14,15	0.56	0	17,19,21	0.87	0
4	PE3	B	1551	-	6,6,42	0.52	0	5,5,41	1.40	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
3	NAG	A	1544	1	1/1/5/7	2/6/23/26	0/1/1/1
5	EDO	B	1549	-	-	1/1/1/1	-
4	PE3	B	1550	-	-	1/1/1/40	-
5	EDO	A	1548	-	-	0/1/1/1	-
4	PE3	A	1550	-	-	1/1/1/40	-
3	NAG	B	1548	1	1/1/5/7	3/6/23/26	0/1/1/1
5	EDO	B	1554	-	-	1/1/1/1	-
4	PE3	B	1547	-	-	4/7/7/40	-
3	NAG	A	1547	1	-	0/6/23/26	0/1/1/1
2	5GZ	A	1549	-	-	5/15/17/25	0/2/2/2
2	5GZ	B	1544	-	-	2/23/25/25	0/2/2/2
4	PE3	A	1545	-	-	1/2/2/40	-
4	PE3	A	1546	-	-	1/4/4/40	-
5	EDO	A	1551	-	-	0/1/1/1	-
4	PE3	A	1553	-	-	3/7/7/40	-
4	PE3	B	1545	-	-	1/4/4/40	-
4	PE3	B	1555	-	-	8/19/19/40	-
4	PE3	B	1553	-	-	1/4/4/40	-
2	5GZ	B	1552	-	-	6/16/18/25	0/2/2/2
4	PE3	A	1552	-	-	2/4/4/40	-
2	5GZ	A	1543	-	-	3/23/25/25	0/2/2/2
3	NAG	B	1546	1	1/1/5/7	3/6/23/26	0/1/1/1
4	PE3	B	1551	-	-	1/4/4/40	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1552	5GZ	S02-N20	5.87	1.70	1.61
2	A	1549	5GZ	C21-N20	5.86	1.52	1.46
2	A	1543	5GZ	C03-S02	-3.65	1.70	1.76
2	B	1544	5GZ	S02-N20	3.61	1.67	1.61
2	B	1552	5GZ	C11-N12	3.61	1.52	1.45
2	B	1544	5GZ	C11-N12	3.41	1.52	1.45
2	B	1544	5GZ	C03-S02	-3.22	1.71	1.76
2	B	1544	5GZ	C22-N23	3.11	1.54	1.47
2	A	1543	5GZ	S02-N20	3.08	1.66	1.61
2	A	1543	5GZ	C22-N23	3.02	1.54	1.47
2	A	1543	5GZ	C18-CL	-2.68	1.67	1.73
2	A	1549	5GZ	C18-CL	-2.11	1.68	1.73
2	A	1549	5GZ	C06-C03	2.09	1.42	1.38



All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1544	5GZ	C04-C03-S02	5.76	126.04	119.77
2	B	1552	5GZ	C04-C03-S02	5.69	125.96	119.77
2	B	1552	5GZ	C06-C03-C04	-5.51	112.75	120.44
2	A	1549	5GZ	C06-C03-C04	-5.39	112.92	120.44
2	A	1543	5GZ	C05-C04-C03	5.21	124.84	119.45
2	B	1552	5GZ	C07-C06-C03	5.07	124.70	119.45
2	A	1549	5GZ	C07-C06-C03	4.87	124.49	119.45
2	A	1549	5GZ	C04-C03-S02	4.85	125.05	119.77
2	A	1549	5GZ	C05-C04-C03	4.85	124.47	119.45
2	B	1552	5GZ	C05-C04-C03	4.81	124.43	119.45
2	B	1544	5GZ	C06-C03-C04	-4.73	113.85	120.44
2	A	1543	5GZ	C06-C03-C04	-4.59	114.04	120.44
2	B	1544	5GZ	C07-C06-C03	4.58	124.19	119.45
2	A	1543	5GZ	C04-C03-S02	4.50	124.67	119.77
2	B	1544	5GZ	C05-C04-C03	4.44	124.05	119.45
2	A	1543	5GZ	C22-C21-N20	4.40	118.60	110.20
3	B	1548	NAG	C3-C4-C5	4.21	117.75	110.24
3	B	1548	NAG	C4-C3-C2	4.18	117.15	111.02
3	A	1547	NAG	C1-O5-C5	3.89	117.46	112.19
2	A	1543	5GZ	C07-C06-C03	3.88	123.46	119.45
2	B	1552	5GZ	C03-S02-N20	3.50	112.41	107.55
2	B	1544	5GZ	C15-C11-N12	-3.32	112.93	116.47
2	B	1544	5GZ	C22-C21-N20	3.19	116.28	110.20
2	B	1552	5GZ	C22-C21-N20	3.08	122.14	111.52
3	B	1548	NAG	C2-N2-C7	2.99	127.15	122.90
2	A	1549	5GZ	C03-S02-N20	2.83	111.47	107.56
3	A	1544	NAG	C1-O5-C5	2.64	115.77	112.19
2	B	1552	5GZ	O28-S02-O01	-2.61	116.34	119.55
2	A	1549	5GZ	O28-S02-O01	-2.61	116.34	119.55
2	A	1549	5GZ	C15-C11-N12	-2.49	113.82	116.47
2	A	1543	5GZ	C08-O09-C10	2.33	122.23	118.48
3	A	1544	NAG	O5-C5-C6	2.26	110.74	107.20
3	B	1548	NAG	O5-C5-C6	2.25	110.73	107.20
3	B	1548	NAG	O5-C1-C2	-2.08	108.00	111.29
2	A	1549	5GZ	C06-C03-S02	2.08	122.03	119.77
2	B	1544	5GZ	O28-S02-O01	-2.07	117.00	119.55

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1544	NAG	C1
3	B	1546	NAG	C1

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Mol	Chain	Res	Type	Atom
3	B	1548	NAG	C1

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1543	5GZ	N20-C21-C22-N23
2	A	1549	5GZ	C21-N20-S02-C03
2	B	1552	5GZ	C22-C21-N20-S02
3	B	1546	NAG	C3-C2-N2-C7
3	B	1546	NAG	C8-C7-N2-C2
3	B	1546	NAG	O7-C7-N2-C2
3	B	1548	NAG	C3-C2-N2-C7
3	B	1548	NAG	C8-C7-N2-C2
3	B	1548	NAG	O7-C7-N2-C2
4	B	1555	PE3	O25-C26-C27-O28
4	A	1553	PE3	O37-C38-C39-O40
4	A	1552	PE3	O37-C38-C39-O40
4	A	1546	PE3	O37-C38-C39-O40
4	B	1547	PE3	O40-C41-C42-O43
2	A	1549	5GZ	C06-C03-S02-O28
4	A	1553	PE3	O34-C35-C36-O37
2	A	1549	5GZ	C04-C03-S02-O28
4	A	1545	PE3	O40-C41-C42-O43
4	B	1551	PE3	O37-C38-C39-O40
4	B	1555	PE3	O40-C41-C42-O43
5	B	1549	EDO	O1-C1-C2-O2
4	B	1555	PE3	O31-C32-C33-O34
2	B	1552	5GZ	C04-C03-S02-O28
2	A	1549	5GZ	C04-C03-S02-N20
4	B	1553	PE3	O37-C38-C39-O40
2	A	1549	5GZ	C06-C03-S02-N20
2	B	1552	5GZ	C06-C03-S02-O28
2	A	1543	5GZ	C21-C22-N23-C24
2	B	1544	5GZ	C21-C22-N23-C24
2	B	1544	5GZ	C21-C22-N23-C26
4	B	1550	PE3	O40-C41-C42-O43
2	B	1552	5GZ	C15-C11-N12-O14
4	A	1552	PE3	C38-C39-O40-C41
4	B	1555	PE3	C29-C30-O31-C32
4	B	1547	PE3	O34-C35-C36-O37
4	B	1547	PE3	C42-C41-O40-C39
4	B	1555	PE3	C30-C29-O28-C27

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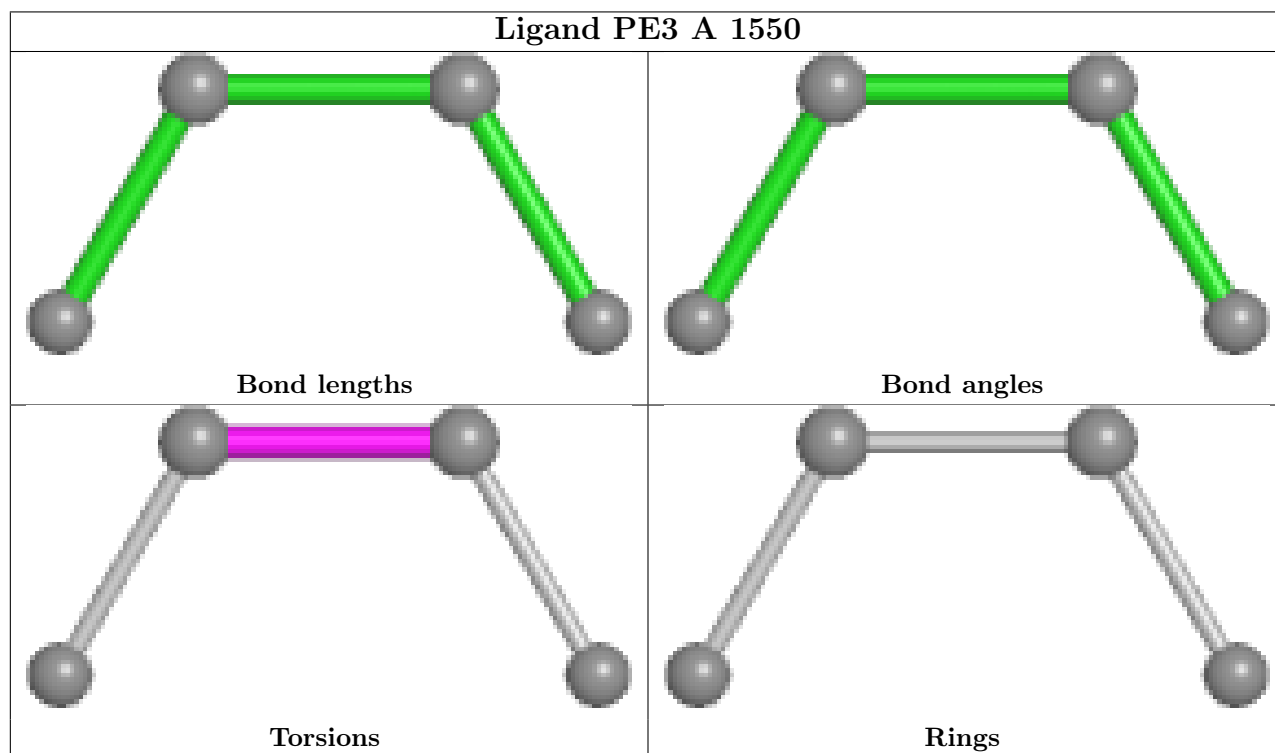
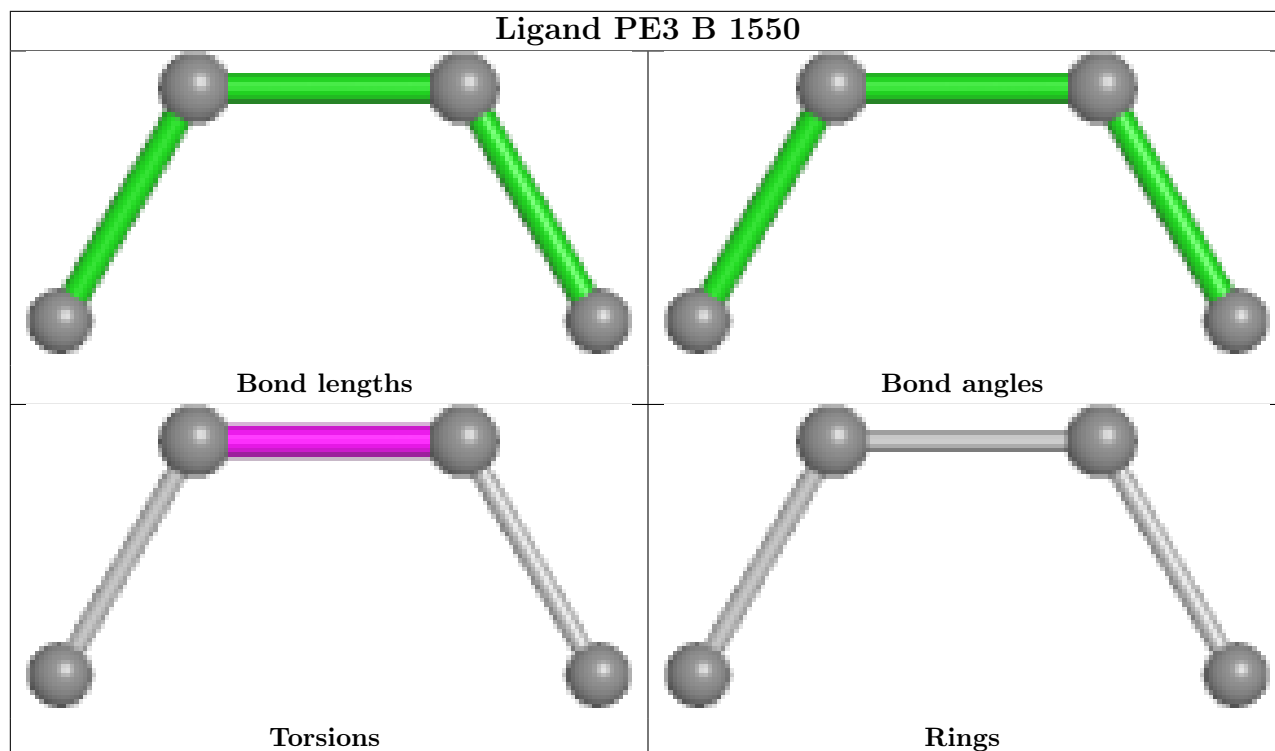
Mol	Chain	Res	Type	Atoms
4	B	1555	PE3	C26-C27-O28-C29
4	B	1545	PE3	O40-C41-C42-O43
4	B	1555	PE3	O22-C23-C24-O25
4	B	1547	PE3	C39-C38-O37-C36
2	A	1543	5GZ	C21-C22-N23-C26
4	B	1555	PE3	O28-C29-C30-O31
4	A	1550	PE3	O40-C41-C42-O43
2	B	1552	5GZ	C04-C03-S02-N20
3	A	1544	NAG	C8-C7-N2-C2
5	B	1554	EDO	O1-C1-C2-O2
3	A	1544	NAG	O7-C7-N2-C2
2	B	1552	5GZ	C06-C03-S02-N20
4	A	1553	PE3	O40-C41-C42-O43

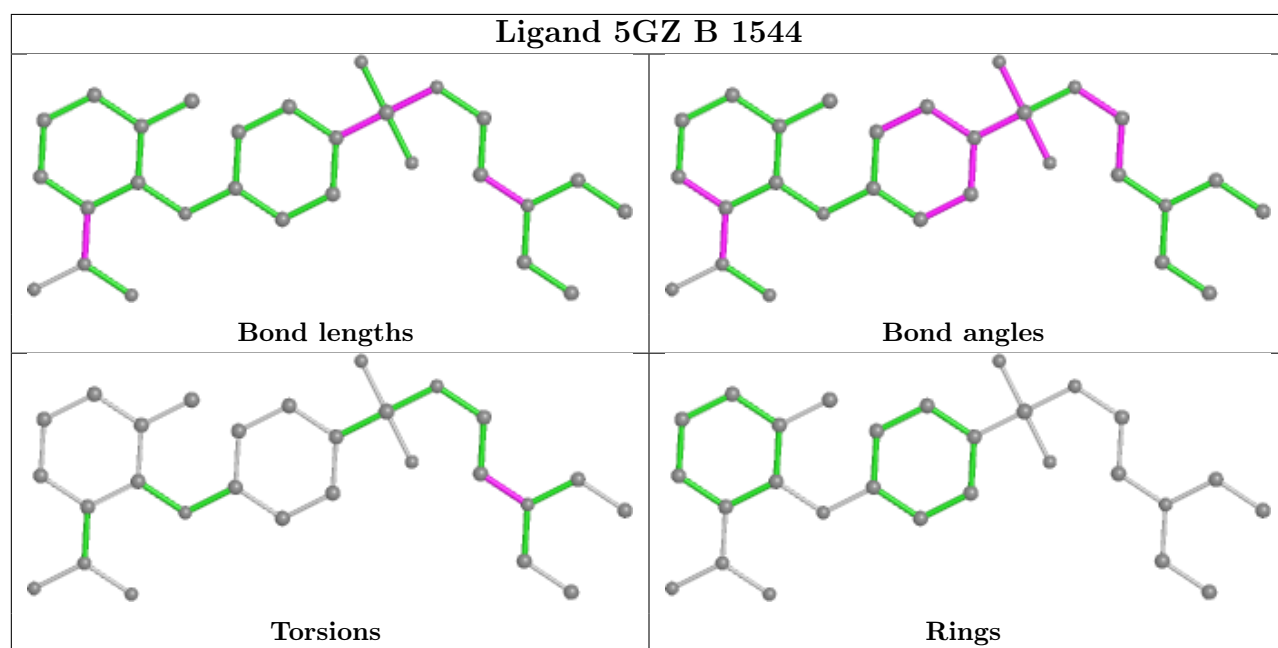
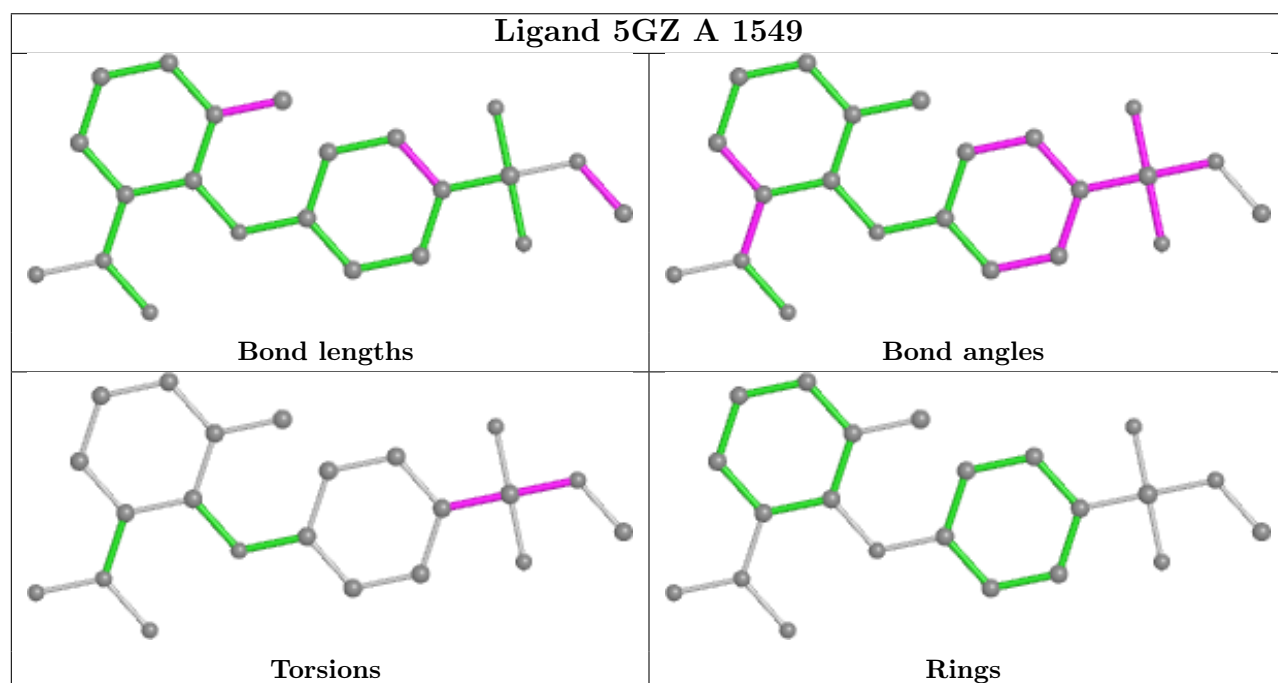
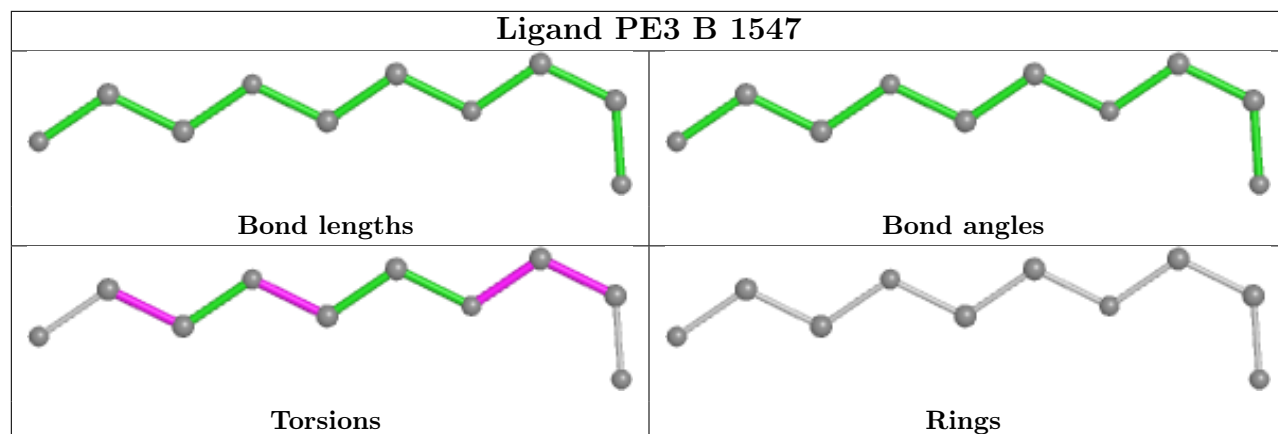
There are no ring outliers.

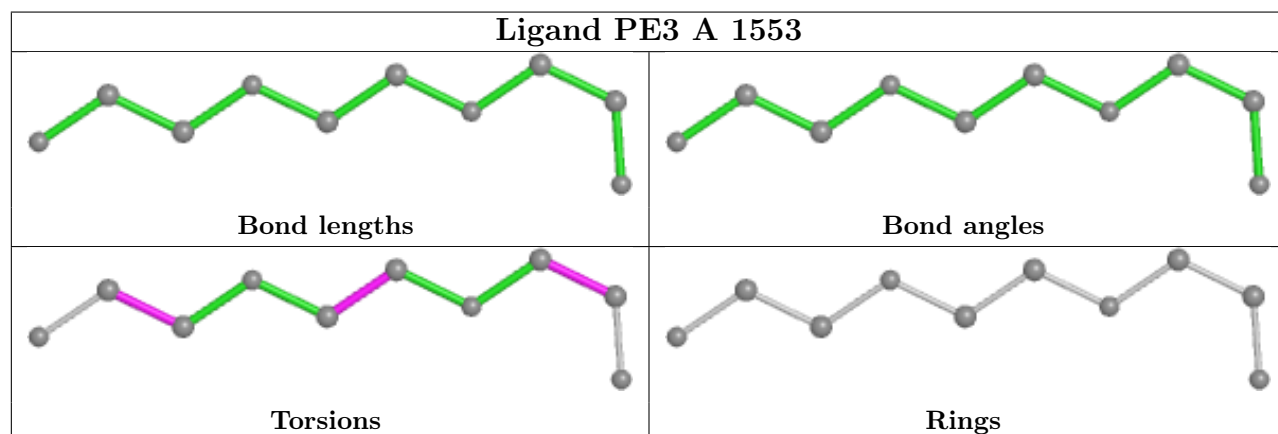
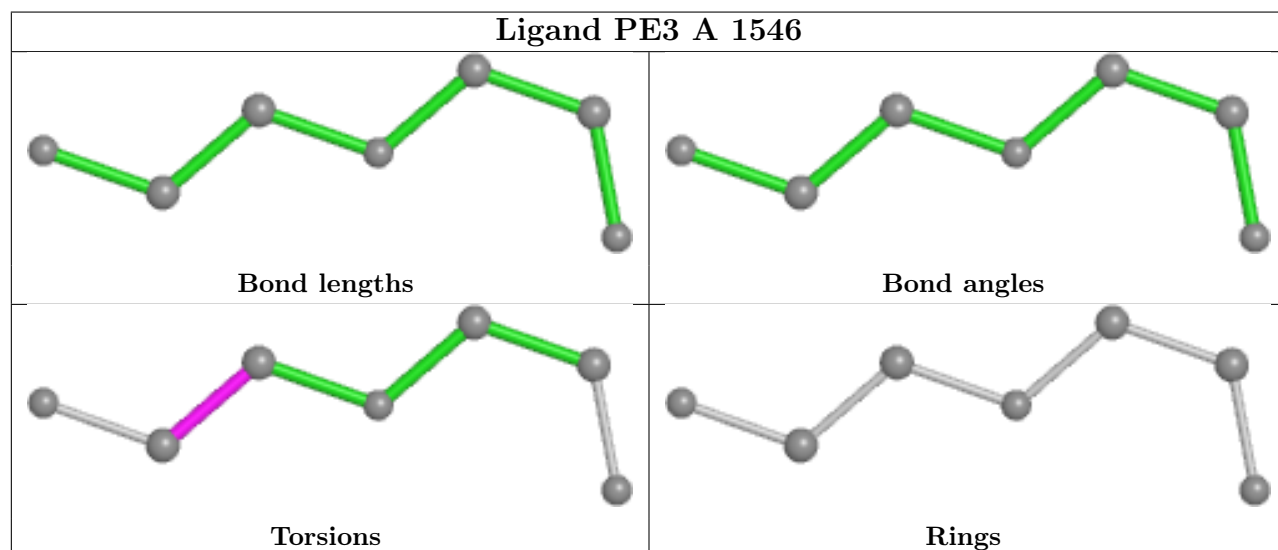
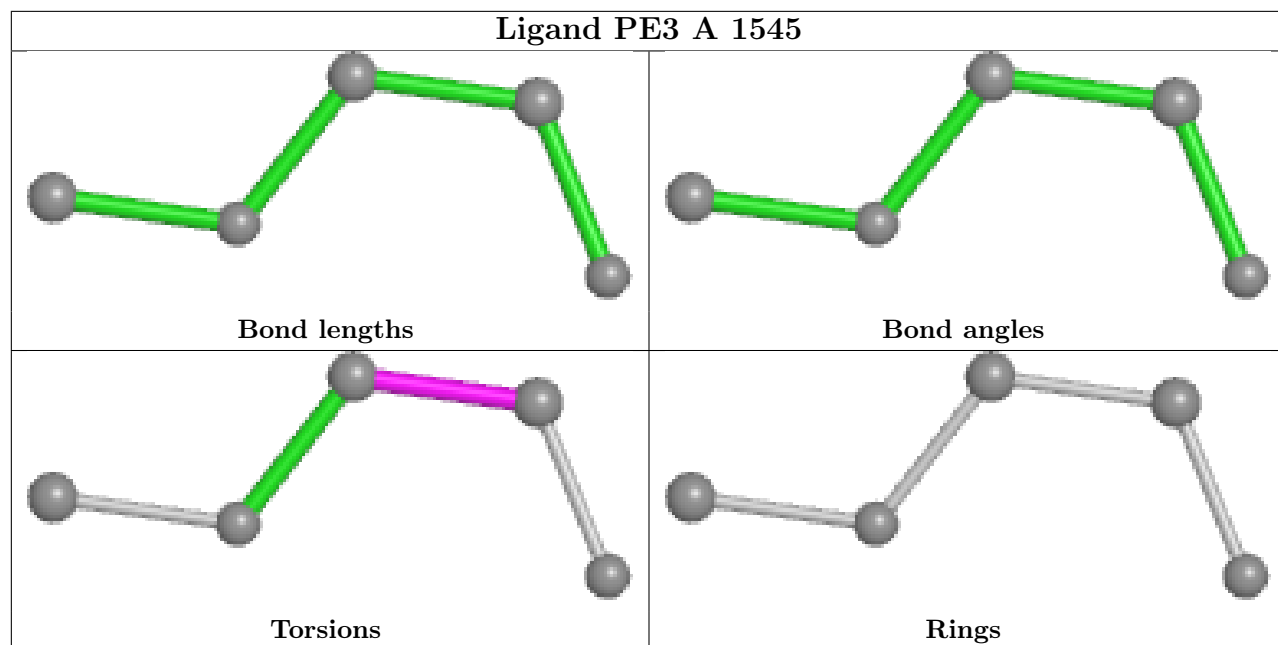
7 monomers are involved in 6 short contacts:

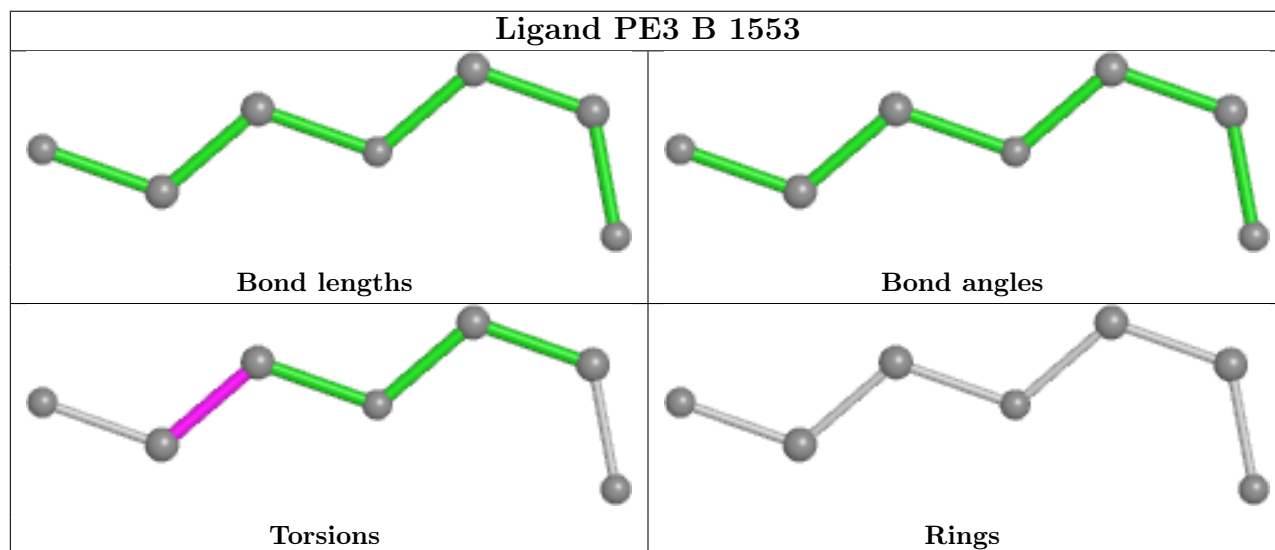
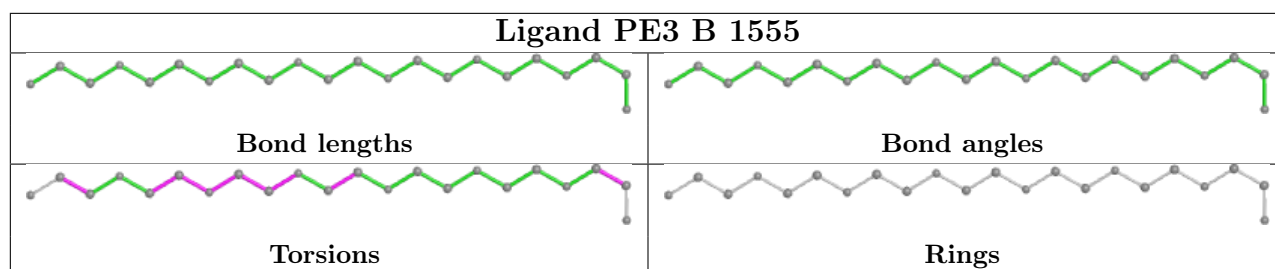
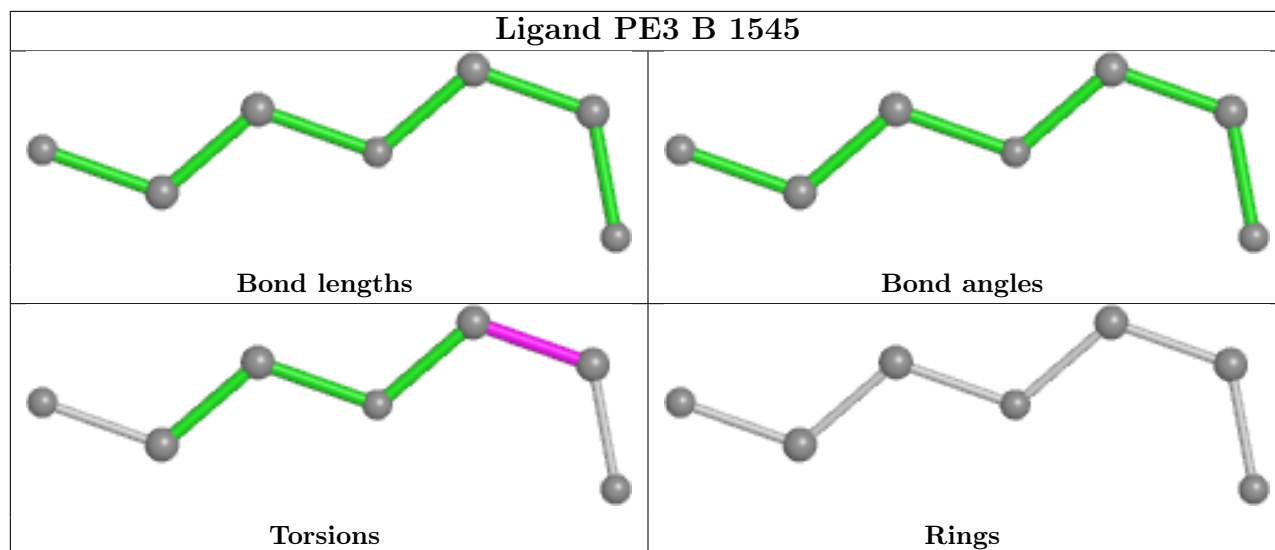
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1549	EDO	2	0
2	A	1549	5GZ	1	0
2	B	1544	5GZ	1	0
4	A	1546	PE3	1	0
4	B	1545	PE3	1	0
4	B	1555	PE3	1	0
2	B	1552	5GZ	1	0

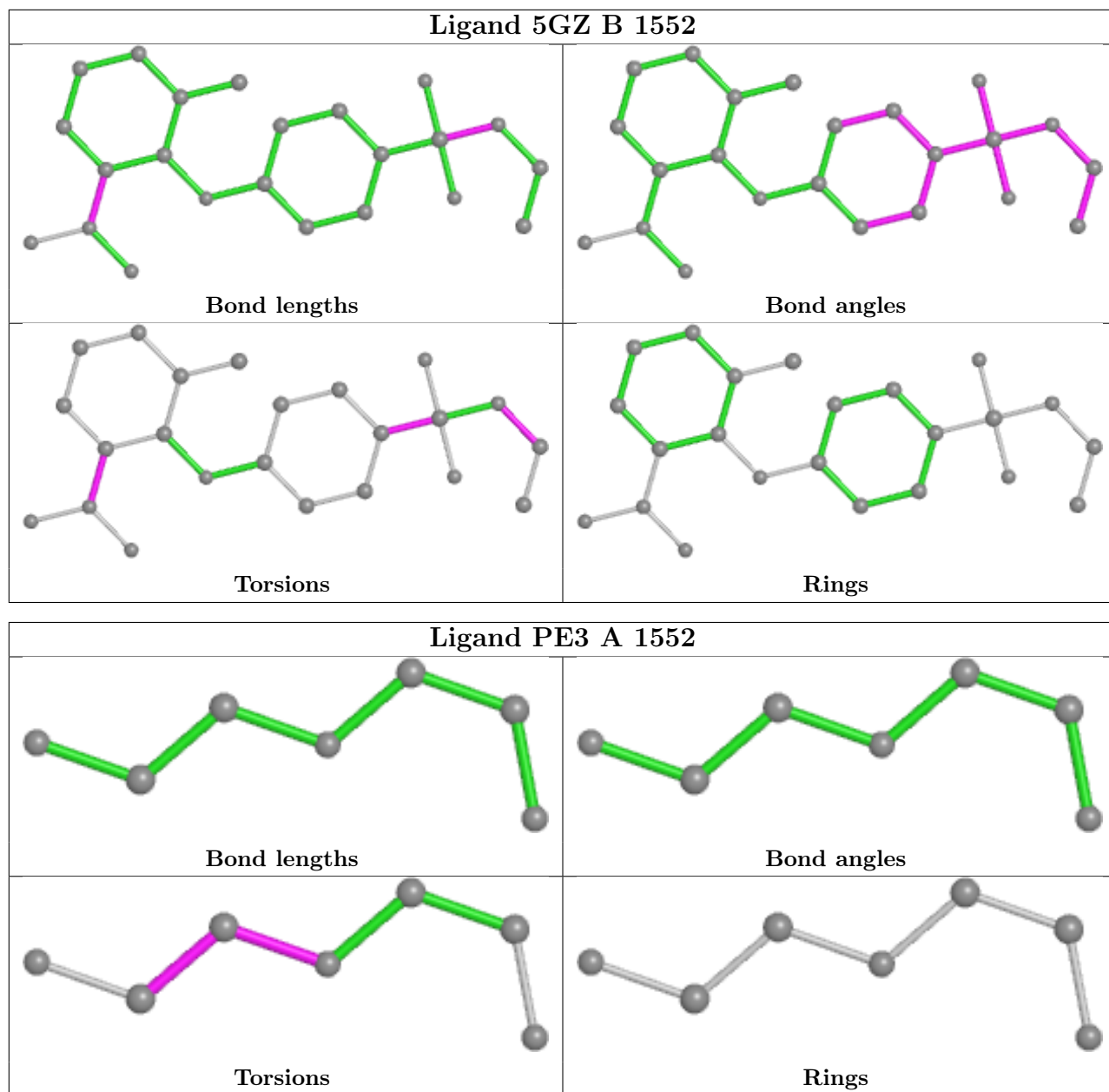
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



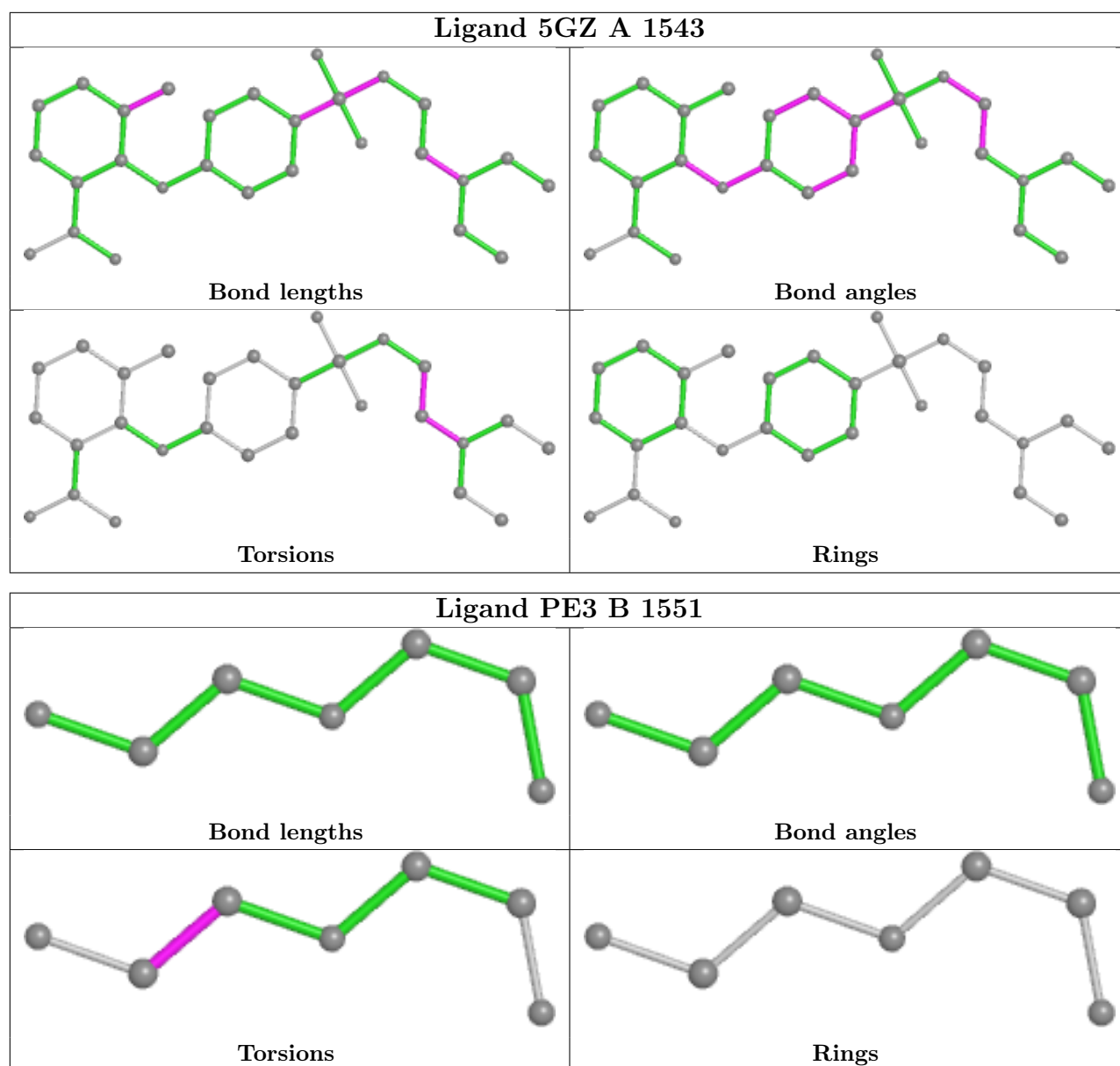












## 5.7 Other polymers [i](#)

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	535/543 (98%)	-0.34	7 (1%) 77 79	30, 48, 78, 136	0
1	B	534/543 (98%)	-0.29	8 (1%) 73 75	37, 54, 84, 148	0
All	All	1069/1086 (98%)	-0.31	15 (1%) 75 77	30, 51, 82, 148	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	543	THR	4.8
1	A	496	LYS	4.7
1	A	540	LEU	3.7
1	A	495	SER	3.4
1	B	497	SER	3.2
1	A	541	SER	2.9
1	B	495	SER	2.9
1	A	494	ASP	2.7
1	B	78	PRO	2.5
1	A	497	SER	2.5
1	B	541	SER	2.4
1	B	79	GLY	2.4
1	A	493	ARG	2.2
1	B	264	GLY	2.1
1	B	105	TYR	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands i

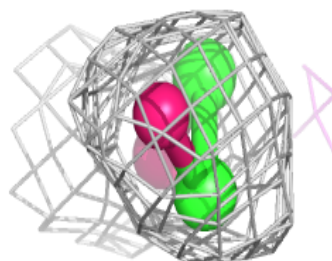
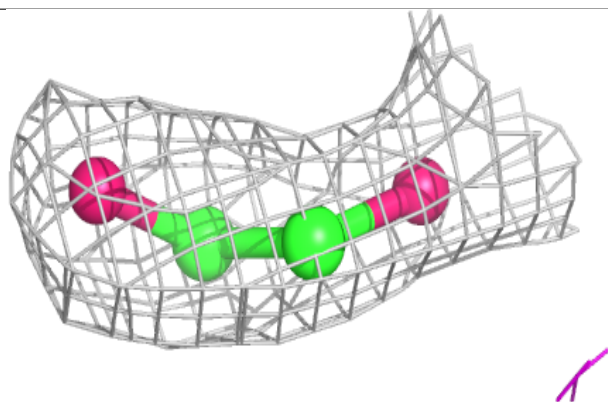
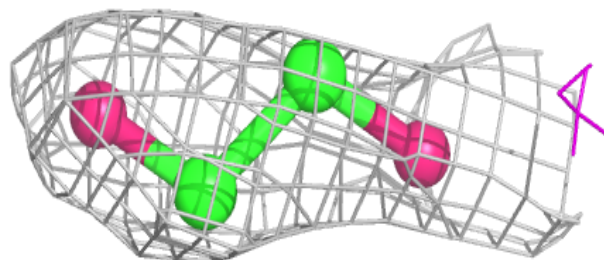
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	1544	14/15	0.54	0.45	94,109,113,115	0
3	NAG	B	1548	14/15	0.58	0.39	84,99,106,106	0
5	EDO	A	1548	4/4	0.74	0.25	76,78,81,84	0
4	PE3	B	1550	4/43	0.78	0.27	77,78,93,95	0
3	NAG	B	1546	14/15	0.78	0.40	108,121,128,129	0
3	NAG	A	1547	14/15	0.82	0.35	90,103,107,107	0
2	5GZ	B	1552	23/28	0.84	0.32	67,92,143,153	23
5	EDO	B	1554	4/4	0.85	0.14	71,72,73,80	0
5	EDO	A	1551	4/4	0.86	0.25	84,85,87,89	0
5	EDO	B	1549	4/4	0.86	0.15	61,61,80,82	0
4	PE3	A	1550	4/43	0.86	0.20	66,67,74,80	0
4	PE3	B	1545	7/43	0.88	0.12	82,88,93,95	0
4	PE3	B	1547	10/43	0.91	0.16	57,70,98,99	0
4	PE3	B	1551	7/43	0.91	0.12	62,71,76,80	0
4	PE3	B	1553	7/43	0.91	0.26	79,86,95,96	0
4	PE3	B	1555	22/43	0.91	0.22	44,73,98,103	0
4	PE3	A	1553	10/43	0.92	0.13	65,70,77,79	0
4	PE3	A	1545	5/43	0.94	0.13	66,66,70,73	0
4	PE3	A	1546	7/43	0.94	0.10	68,77,81,82	0
2	5GZ	A	1549	22/28	0.94	0.23	57,72,90,95	22
4	PE3	A	1552	7/43	0.94	0.25	68,70,85,89	0
2	5GZ	A	1543	28/28	0.94	0.19	19,48,64,108	28
2	5GZ	B	1544	28/28	0.96	0.15	34,54,86,94	0

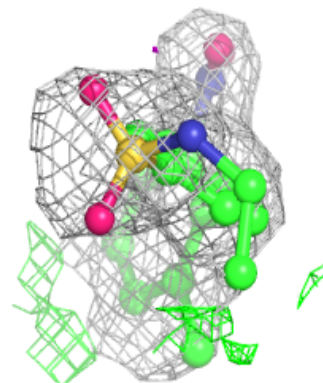
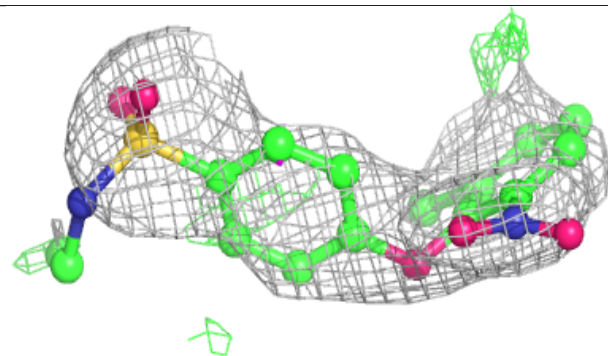
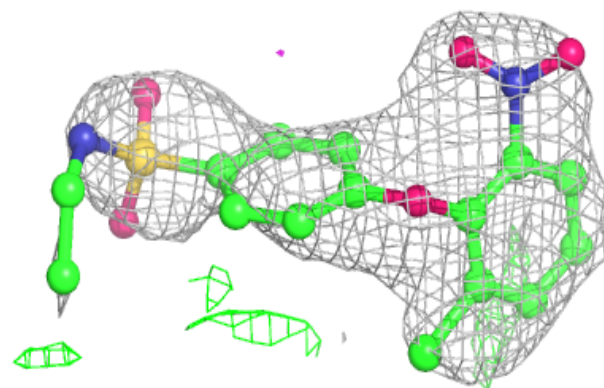
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PE3 B 1550:**

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

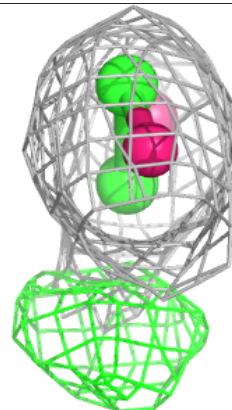
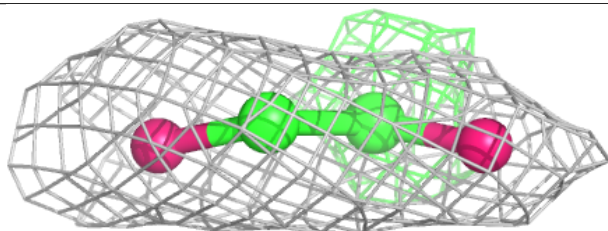
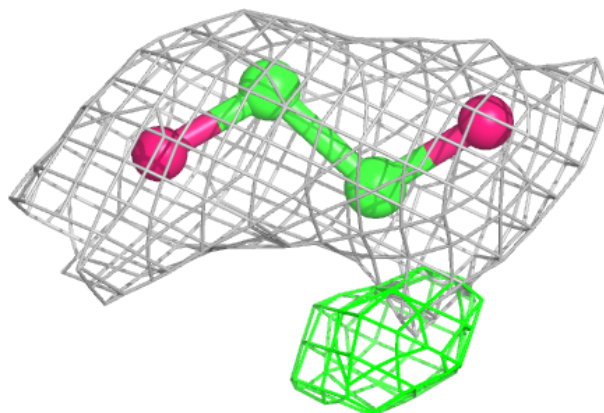
**Electron density around 5GZ B 1552:**

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

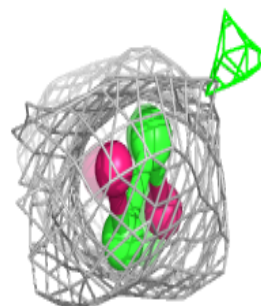
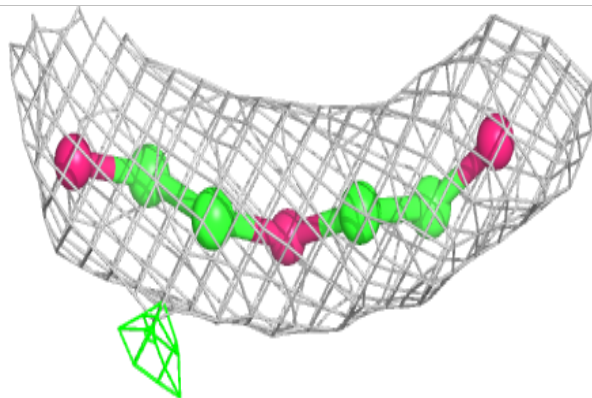
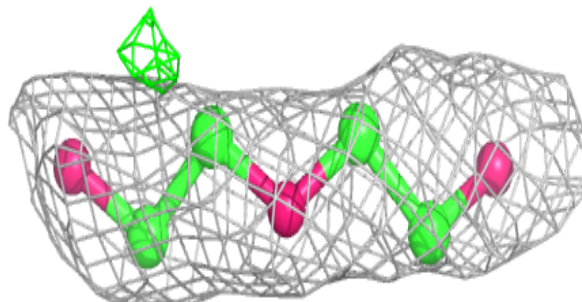


**Electron density around PE3 A 1550:**

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

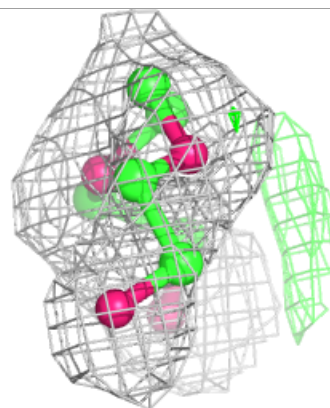
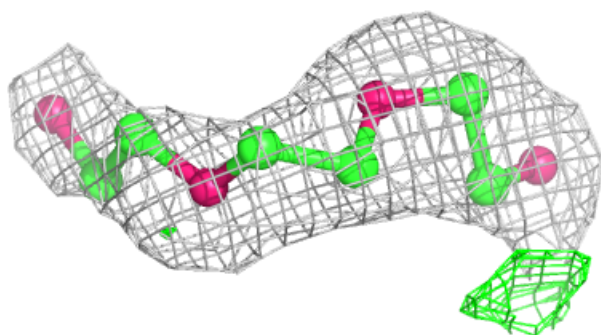
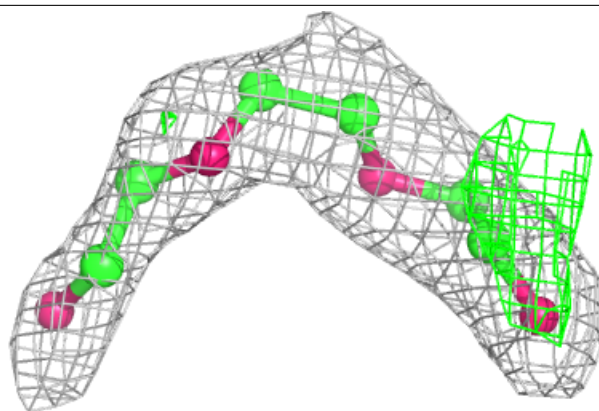
**Electron density around PE3 B 1545:**

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

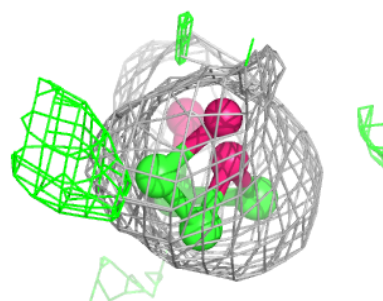
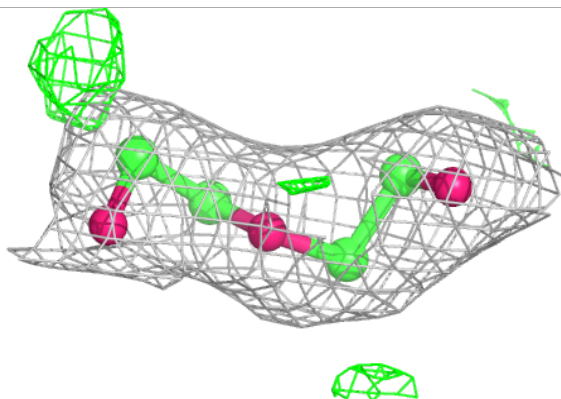
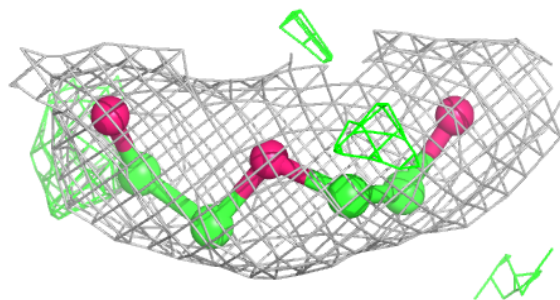


**Electron density around PE3 B 1547:**

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

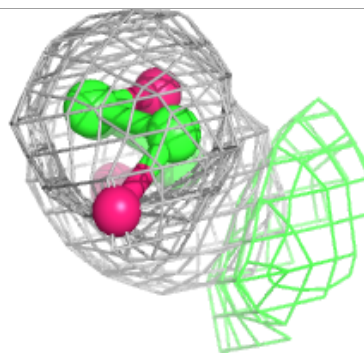
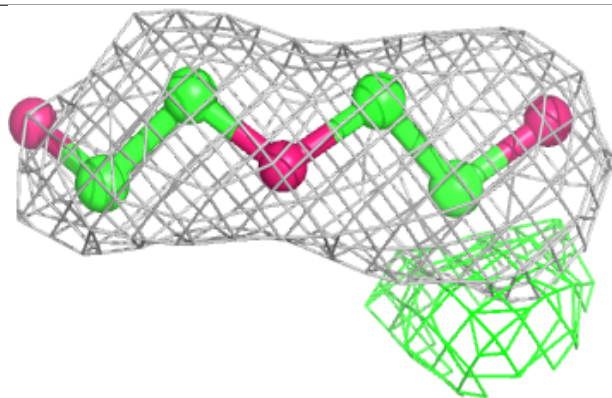
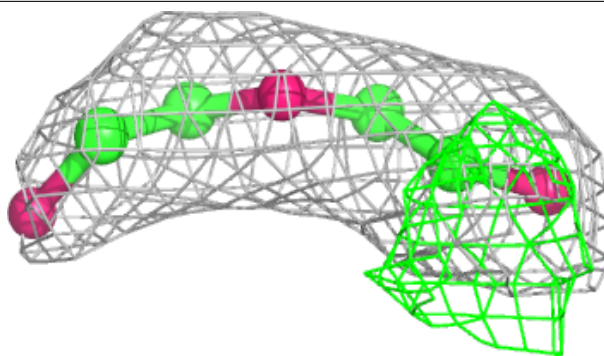
**Electron density around PE3 B 1551:**

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



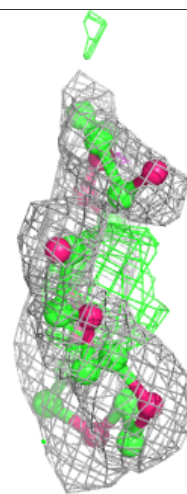
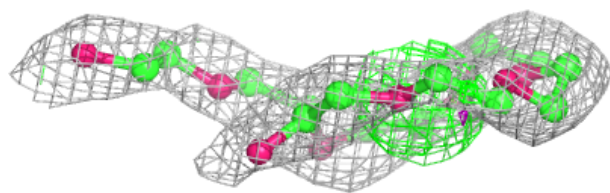
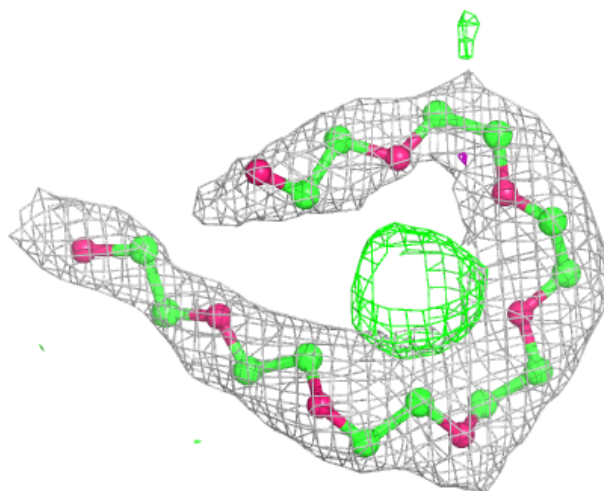
**Electron density around PE3 B 1553:**

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



**Electron density around PE3 B 1555:**

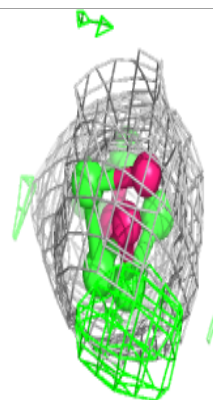
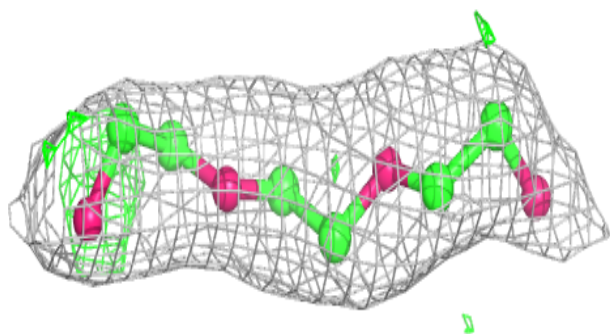
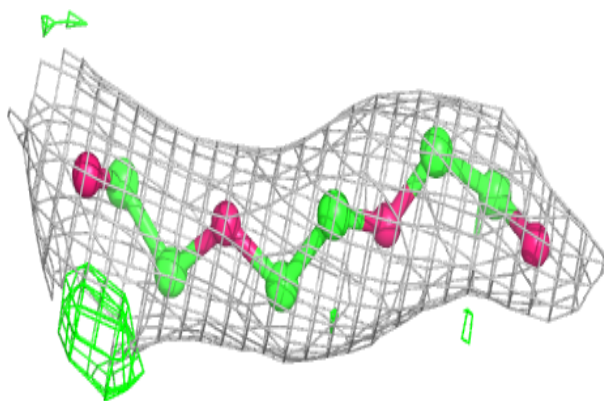
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



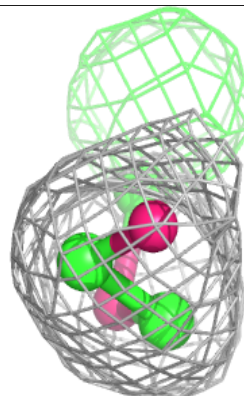
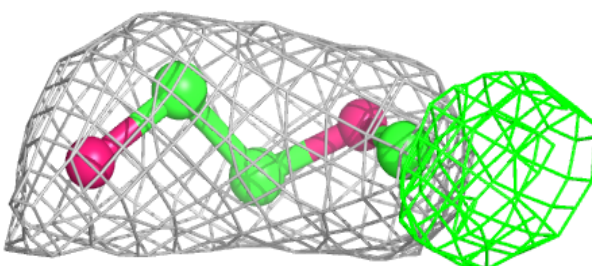
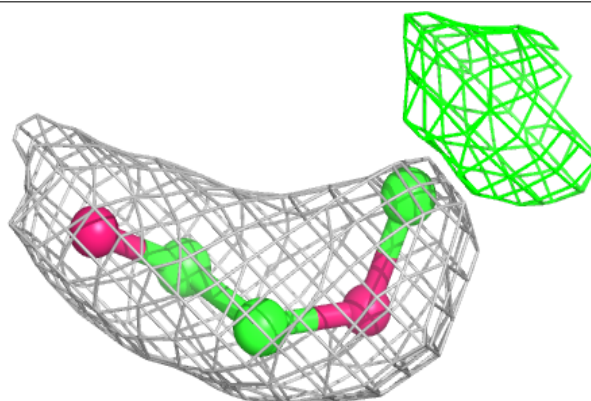


**Electron density around PE3 A 1553:**

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

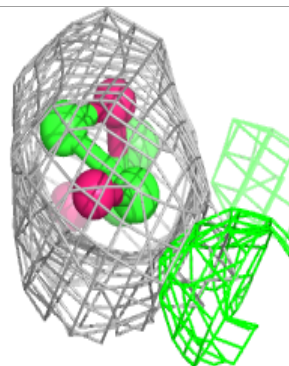
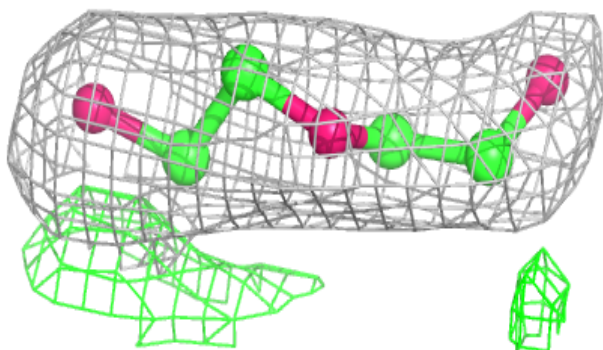
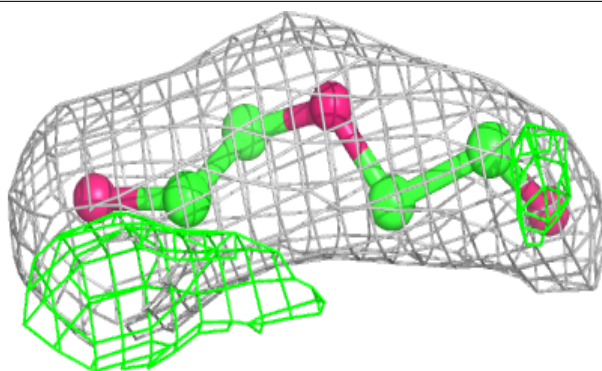
**Electron density around PE3 A 1545:**

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

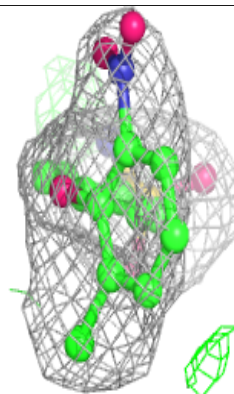
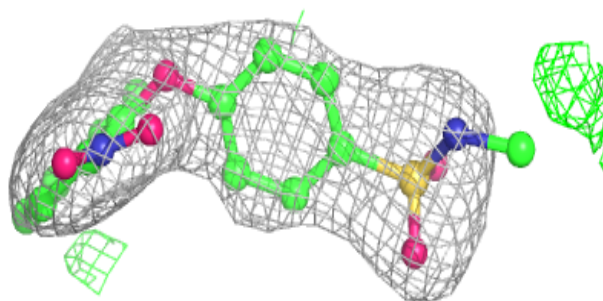
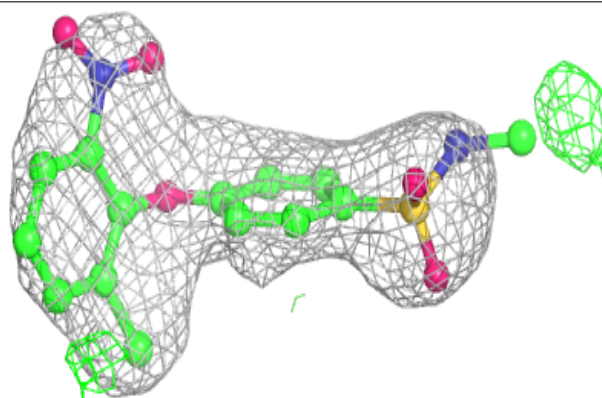


**Electron density around PE3 A 1546:**

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

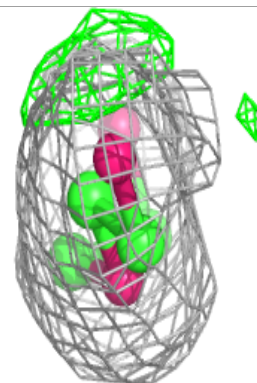
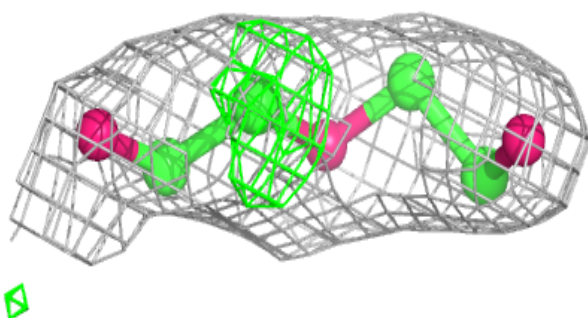
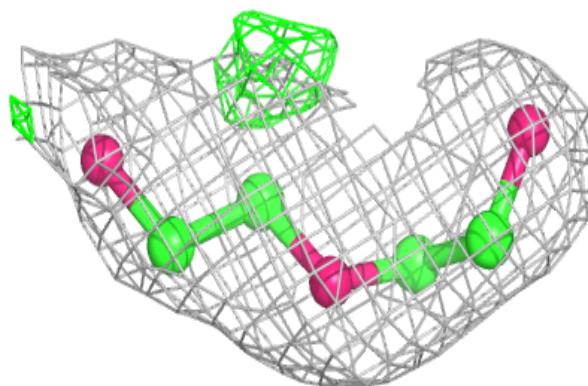
**Electron density around 5GZ A 1549:**

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

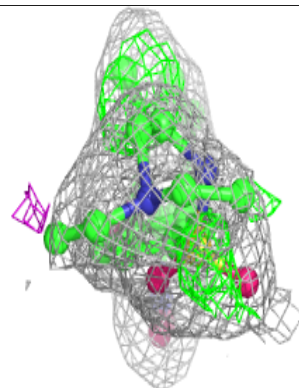
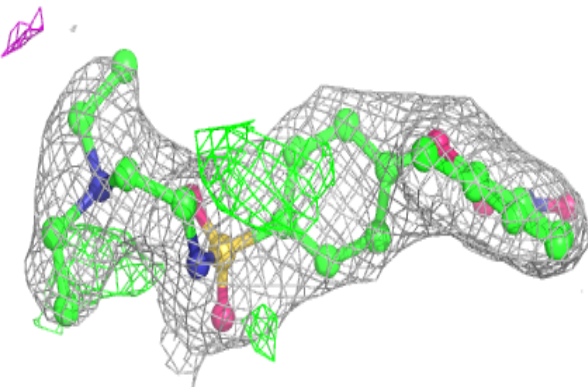
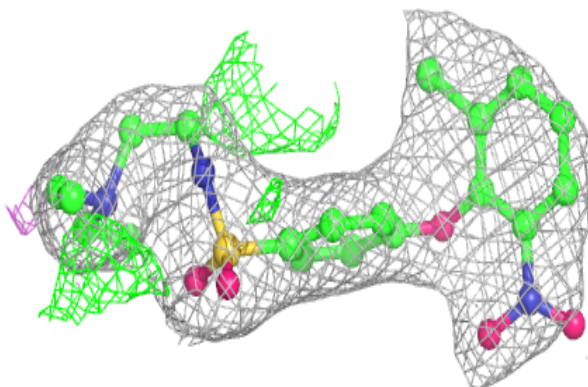


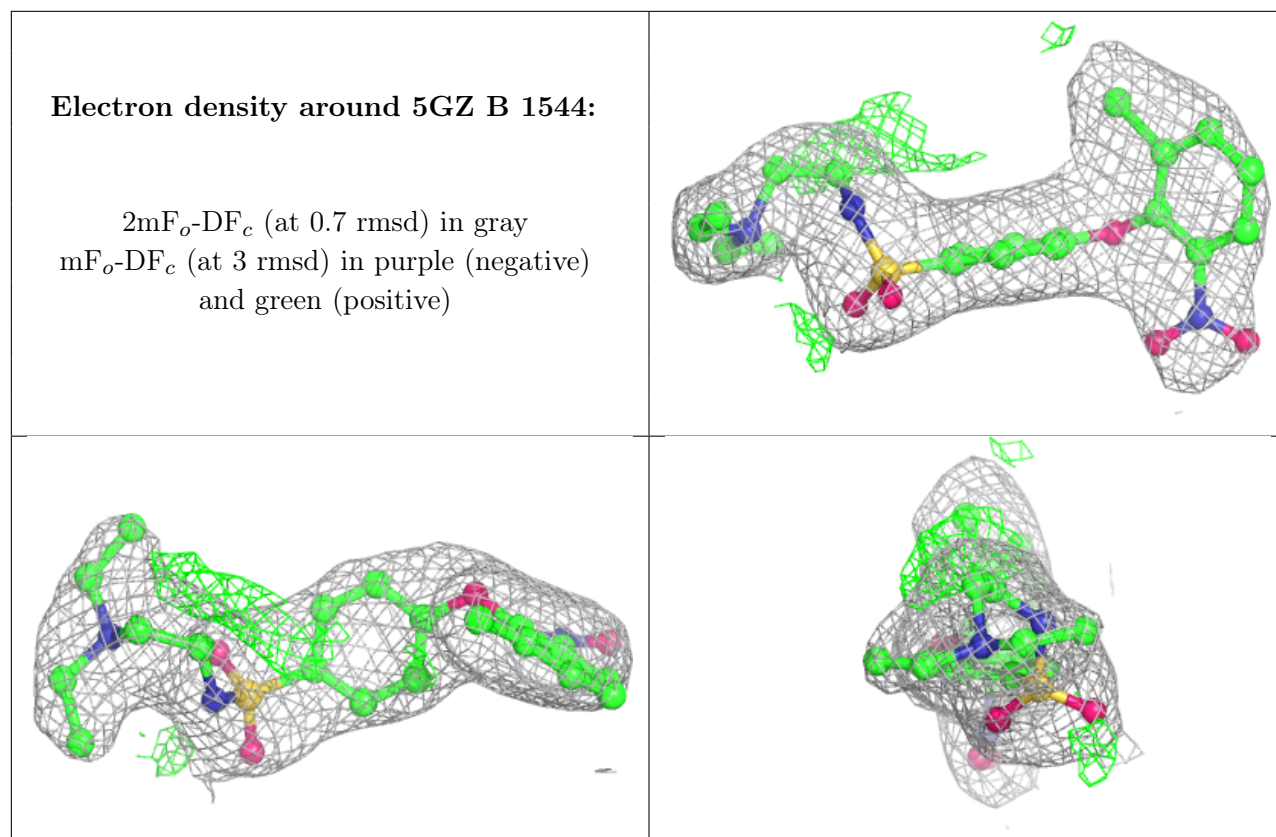
**Electron density around PE3 A 1552:**

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

**Electron density around 5GZ A 1543:**

$2mF_o-DF_c$  (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.