



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:15 PM UTC

PDB ID : 2YEQ / pdb_00002yeq
Title : Structure of PhoD
Authors : Lillington, J.E.D.; Rodriguez, F.; Roversi, P.; Johnson, S.J.; Berks, B.; Lea, S.M.
Deposited on : 2011-03-30
Resolution : 1.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

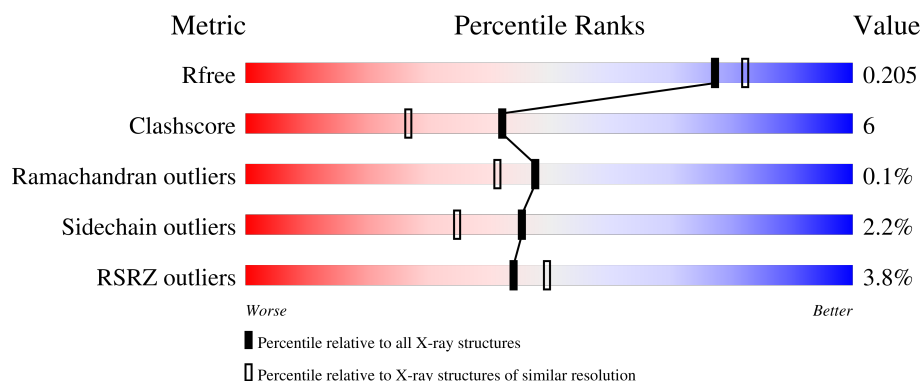
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	
1	B	527	

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	EDO	A	539	-	-	X	-
3	EDO	A	566	-	-	X	-
3	EDO	A	569	-	-	X	-
3	EDO	A	579	-	-	X	-

2 Entry composition ⓘ

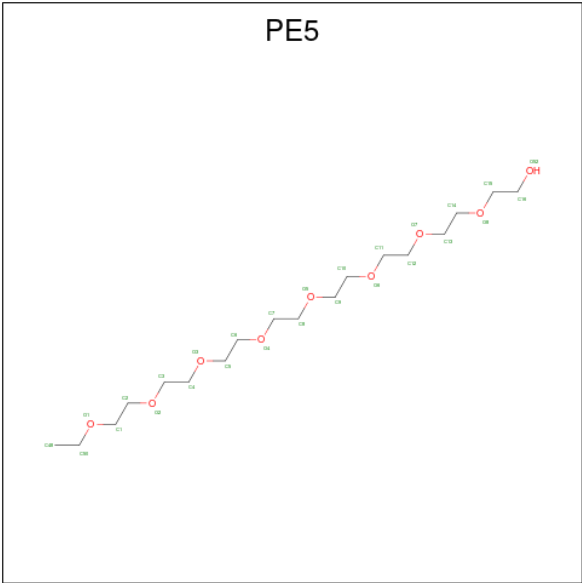
There are 8 unique types of molecules in this entry. The entry contains 9447 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALKALINE PHOSPHATASE D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4187	2649	741	786	11			
1	B	522	Total	C	N	O	S	0	1	0
			4193	2653	742	787	11			

- Molecule 2 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (CCD ID: PE5) (formula: C₁₈H₃₈O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			7	5	2		
2	A	1	Total	C	O	0	0
			6	4	2		
2	A	1	Total	C	O	0	0
			16	11	5		

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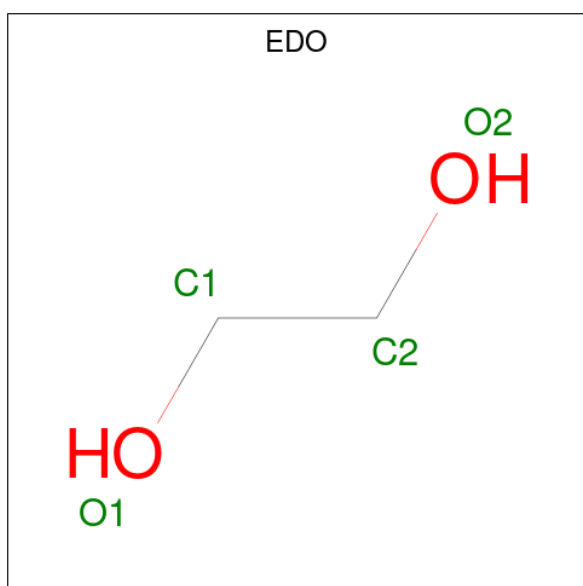
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	4	2		
2	A	1	Total	C	O	0	0
			8	5	3		
2	A	1	Total	C	O	0	0
			7	5	2		
2	A	1	Total	C	O	0	0
			4	3	1		
2	A	1	Total	C	O	0	0
			6	4	2		
2	A	1	Total	C	O	0	0
			7	5	2		
2	A	1	Total	C	O	0	0
			7	5	2		
2	A	1	Total	C	O	0	0
			12	8	4		
2	A	1	Total	C	O	0	0
			7	5	2		
2	A	1	Total	C	O	0	0
			7	5	2		
2	B	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			7	5	2		
2	B	1	Total	C	O	0	0
			6	4	2		
2	B	1	Total	C	O	0	0
			16	11	5		
2	B	1	Total	C	O	0	0
			6	4	2		
2	B	1	Total	C	O	0	0
			15	10	5		
2	B	1	Total	C	O	0	0
			8	5	3		
2	B	1	Total	C	O	0	0
			7	5	2		
2	B	1	Total	C	O	0	0
			4	3	1		
2	B	1	Total	C	O	0	0
			6	4	2		
2	B	1	Total	C	O	0	0
			7	5	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			7	5	2		
2	B	1	Total	C	O	0	0
			7	5	2		
2	B	1	Total	C	O	0	0
			8	5	3		
2	B	1	Total	C	O	0	0
			7	5	2		
2	B	1	Total	C	O	0	0
			7	5	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	1
			8	4	4		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Na 3 3	0	0
4	B	3	Total Na 3 3	0	0

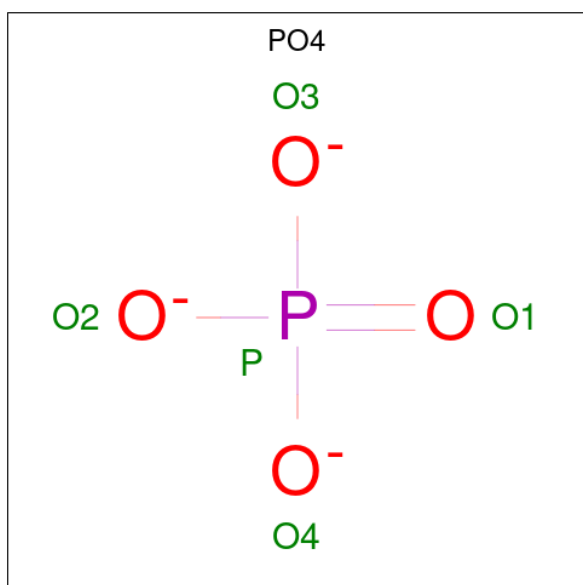
- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe 1 1	0	0
5	B	1	Total Fe 1 1	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Ca 2 2	0	0
6	B	2	Total Ca 2 2	0	0

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O P 5 4 1	0	0
7	B	1	Total O P 5 4 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	325	Total O 325 325	0	0

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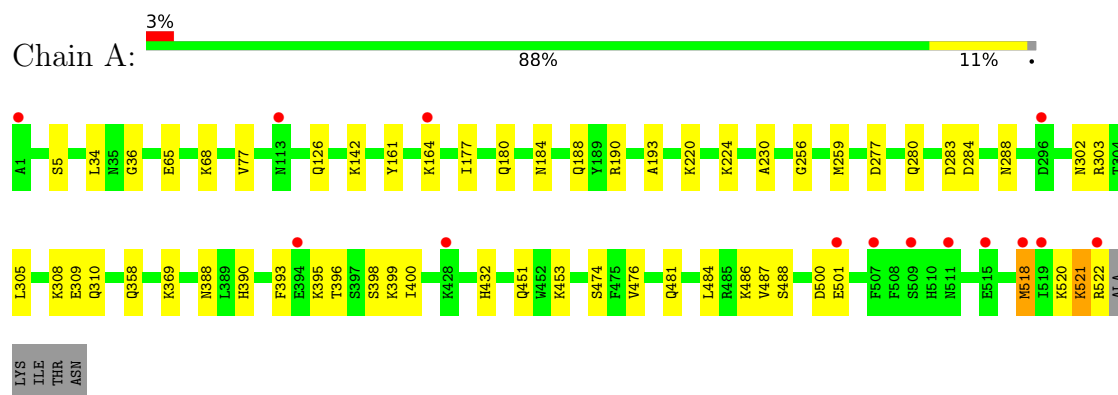
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	300	Total 300	O 300	0	0

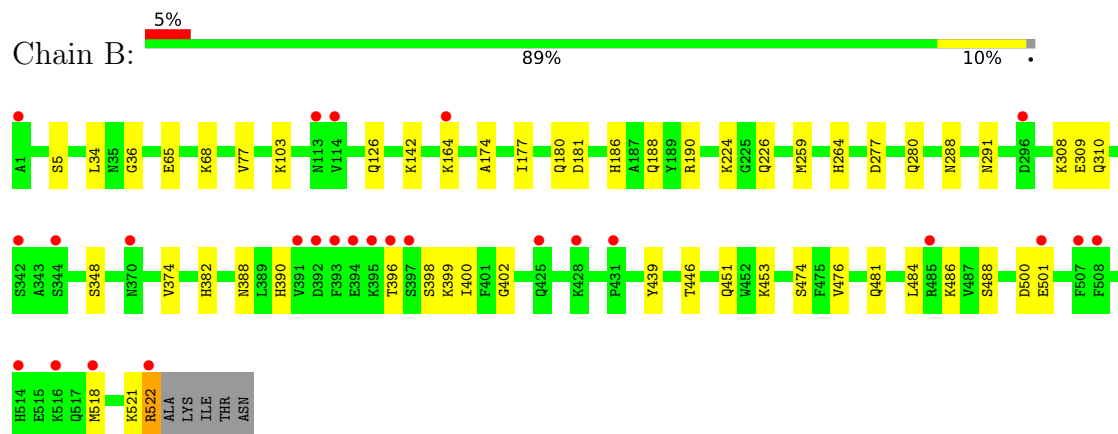
3 Residue-property plots

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: ALKALINE PHOSPHATASE D



• Molecule 1: ALKALINE PHOSPHATASE D



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	147.32Å 147.32Å 347.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	135.64 – 1.93 135.64 – 1.93	Depositor EDS
% Data completeness (in resolution range)	98.8 (135.64-1.93) 98.9 (135.64-1.93)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.92Å)	Xtrriage
Refinement program	REFMAC 5.6.0095	Depositor
R, R_{free}	0.178 , 0.202 0.183 , 0.205	Depositor DCC
R_{free} test set	7130 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtrriage
Anisotropy	0.107	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9447	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 43.66 % 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 1.7077e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NA, FE, CA, PO4, PE5

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	0.78	0/4306	0.78	0/5845
1	B	0.74	0/4312	0.77	0/5852
All	All	0.76	0/8618	0.77	0/11697

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	4187	0	4006	57	0
1	B	4193	0	4009	44	0
2	A	113	0	124	17	0
2	B	131	0	145	18	0
3	A	92	0	138	22	0
3	B	84	0	126	7	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	2	0	0	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
8	A	325	0	0	12	0
8	B	300	0	0	10	0
All	All	9447	0	8548	110	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 6.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LYS:H	2:A:554:PE5:H482	1.30	0.96
1:B:224:LYS:H	2:B:554:PE5:H482	1.32	0.94
2:B:534:PE5:H482	8:B:2244:HOH:O	1.72	0.88
1:A:518:MET:HE2	8:B:2181:HOH:O	1.77	0.84
1:A:388:ASN:HD21	1:A:484:LEU:H	1.19	0.84
1:B:388:ASN:HD21	1:B:484:LEU:H	1.24	0.80
1:B:277:ASP:H	1:B:310:GLN:HE22	1.28	0.79
2:A:581:PE5:C4	8:A:2065:HOH:O	2.29	0.79
1:A:277:ASP:H	1:A:310:GLN:HE22	1.28	0.78
2:A:546:PE5:C50	8:A:2055:HOH:O	2.32	0.77
1:A:400:ILE:H	1:A:481:GLN:HE22	1.32	0.76
1:A:259:MET:H	1:A:280:GLN:HE22	1.34	0.76
1:B:399:LYS:NZ	8:B:2225:HOH:O	2.15	0.75
1:B:259:MET:H	1:B:280:GLN:HE22	1.35	0.74
1:B:181:ASP:OD1	3:B:565:EDO:H12	1.88	0.73
1:B:400:ILE:H	1:B:481:GLN:HE22	1.34	0.72
1:B:451:GLN:HE22	2:B:534:PE5:H51	1.52	0.72
1:A:302:ASN:HD21	2:B:536:PE5:H483	1.55	0.71
1:A:369:LYS:HZ3	2:A:529:PE5:H42	1.58	0.69
3:A:539:EDO:H22	1:B:226:GLN:O	1.94	0.68
1:B:451:GLN:HE22	2:B:534:PE5:C5	2.08	0.65
2:A:581:PE5:C50	8:A:2325:HOH:O	2.45	0.64
1:A:390:HIS:HE1	8:A:2232:HOH:O	1.82	0.62
1:A:399:LYS:NZ	8:A:2238:HOH:O	2.32	0.61
2:A:554:PE5:H483	8:A:2177:HOH:O	1.99	0.61
1:A:284:ASP:HB3	3:A:539:EDO:H21	1.83	0.60
1:A:288:ASN:HD21	1:B:288:ASN:HD21	1.49	0.60
1:B:481:GLN:OE1	8:B:2261:HOH:O	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LYS:NZ	2:B:581:PE5:H12	2.16	0.59
2:B:534:PE5:C9	8:B:2244:HOH:O	2.51	0.58
1:A:220:LYS:HE2	8:A:2153:HOH:O	2.01	0.58
1:B:103:LYS:HZ3	2:B:581:PE5:H12	1.69	0.58
1:A:388:ASN:HD21	1:A:484:LEU:N	1.98	0.58
1:A:453:LYS:NZ	2:A:534:PE5:H72	2.19	0.58
2:B:534:PE5:C48	8:B:2244:HOH:O	2.42	0.58
2:A:534:PE5:H482	8:A:2307:HOH:O	2.03	0.57
1:A:453:LYS:HZ3	2:A:534:PE5:H72	1.69	0.57
1:B:486:LYS:NZ	8:B:2266:HOH:O	2.38	0.56
1:B:34:LEU:HD11	1:B:188:GLN:HA	1.87	0.56
1:B:68:LYS:HZ1	2:B:580:PE5:C2	2.18	0.56
1:A:451:GLN:HE22	2:A:534:PE5:C4	2.19	0.56
1:A:256:GLY:H	3:A:564:EDO:C1	2.19	0.55
1:B:451:GLN:HG3	1:B:476:VAL:CG1	2.37	0.55
1:B:388:ASN:HD21	1:B:484:LEU:N	2.02	0.54
1:A:451:GLN:HG3	1:A:476:VAL:CG1	2.38	0.54
1:A:487:VAL:CG2	2:A:534:PE5:H71	2.37	0.54
1:A:487:VAL:HG21	2:A:534:PE5:H71	1.90	0.54
1:A:193:ALA:HB2	3:A:569:EDO:H21	1.90	0.53
1:B:224:LYS:N	2:B:554:PE5:H482	2.13	0.53
1:B:451:GLN:HG3	1:B:476:VAL:HG13	1.92	0.52
1:A:68:LYS:HZ1	2:A:580:PE5:C1	2.23	0.51
1:A:486:LYS:NZ	3:A:566:EDO:H12	2.26	0.51
1:A:451:GLN:CG	1:A:476:VAL:HG13	2.41	0.51
1:A:220:LYS:CE	8:A:2153:HOH:O	2.56	0.51
1:A:34:LEU:HD11	1:A:188:GLN:HA	1.92	0.50
1:A:193:ALA:H	3:A:569:EDO:C2	2.25	0.50
1:A:283:ASP:HB3	3:A:539:EDO:H12	1.93	0.49
1:B:451:GLN:CG	1:B:476:VAL:HG13	2.43	0.49
1:A:520:LYS:C	1:A:522:ARG:H	2.20	0.49
1:A:451:GLN:HG3	1:A:476:VAL:HG13	1.95	0.48
1:A:303:ARG:HE	3:A:539:EDO:C1	2.27	0.48
1:A:486:LYS:NZ	8:A:2286:HOH:O	2.43	0.48
1:B:186:HIS:HE1	8:B:2126:HOH:O	1.96	0.48
1:B:291:ASN:HD22	1:B:348:SER:HA	1.78	0.48
1:A:396:THR:CG2	3:A:579:EDO:H21	2.43	0.48
1:B:5:SER:H	2:B:557:PE5:C4	2.27	0.48
1:B:439:TYR:OH	3:B:541:EDO:H12	2.14	0.47
1:B:522:ARG:CG	1:B:522:ARG:HH11	2.28	0.47
1:A:256:GLY:H	3:A:564:EDO:H11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ILE:HD12	2:B:536:PE5:H21	1.97	0.46
2:B:581:PE5:H31	8:B:2085:HOH:O	2.15	0.46
1:B:36:GLY:HA2	1:B:180:GLN:HE21	1.80	0.46
1:B:446:THR:HG21	2:B:534:PE5:H22	1.97	0.46
1:A:396:THR:HG23	3:A:579:EDO:H21	1.97	0.46
1:A:161:TYR:OH	3:A:552:EDO:H21	2.17	0.45
1:A:184:ASN:ND2	3:A:565:EDO:H11	2.32	0.45
1:B:451:GLN:NE2	2:B:534:PE5:C5	2.79	0.45
1:B:474:SER:HB3	1:B:488:SER:HB3	1.99	0.45
1:A:284:ASP:CB	3:A:539:EDO:H21	2.48	0.44
1:A:193:ALA:H	3:A:569:EDO:H21	1.83	0.44
1:A:256:GLY:H	3:A:564:EDO:H12	1.83	0.44
1:A:393:PHE:O	3:A:579:EDO:H11	2.18	0.44
1:B:174:ALA:HB3	3:B:550:EDO:H22	2.00	0.43
1:A:193:ALA:CB	3:A:569:EDO:H21	2.47	0.43
1:A:395:LYS:O	1:A:398:SER:OG	2.34	0.43
1:A:486:LYS:NZ	3:A:566:EDO:C1	2.81	0.43
1:A:36:GLY:HA2	1:A:180:GLN:HE21	1.84	0.43
1:A:474:SER:HB3	1:A:488:SER:HB3	2.02	0.42
1:A:5:SER:H	2:A:557:PE5:C4	2.32	0.42
1:A:65:GLU:HG3	1:A:77:VAL:HG22	2.02	0.42
1:B:374:VAL:O	1:B:402:GLY:HA3	2.19	0.42
1:B:65:GLU:HG3	1:B:77:VAL:HG22	2.02	0.41
1:B:451:GLN:NE2	2:B:534:PE5:C4	2.83	0.41
2:A:534:PE5:C9	8:A:2307:HOH:O	2.67	0.41
1:B:396:THR:HG23	3:B:579:EDO:H22	2.02	0.41
1:B:481:GLN:NE2	8:B:2260:HOH:O	2.34	0.41
1:A:177:ILE:HD12	2:A:536:PE5:H21	2.01	0.41
1:B:382:HIS:HD1	3:B:552:EDO:C2	2.33	0.41
1:B:439:TYR:OH	3:B:541:EDO:C1	2.68	0.41
1:B:453:LYS:HZ3	2:B:534:PE5:H61	1.85	0.41
1:A:432:HIS:HB3	3:A:579:EDO:H22	2.03	0.41
1:A:481:GLN:OE1	8:A:2281:HOH:O	2.22	0.41
1:A:486:LYS:HZ2	3:A:566:EDO:H12	1.86	0.41
1:A:305:LEU:HB2	1:A:358:GLN:HG2	2.02	0.41
1:B:521:LYS:O	1:B:522:ARG:C	2.64	0.41
1:B:390:HIS:HD2	1:B:398:SER:O	2.04	0.41
1:A:486:LYS:HZ2	3:A:566:EDO:C1	2.33	0.40
1:A:230:ALA:HB1	2:A:536:PE5:H12	2.04	0.40
1:A:451:GLN:CG	1:A:476:VAL:CG1	2.97	0.40
1:B:264:HIS:NE2	3:B:576:EDO:H11	2.37	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	520/527 (99%)	502 (96%)	17 (3%)	1 (0%)	43	37
1	B	521/527 (99%)	504 (97%)	17 (3%)	0	100	100
All	All	1041/1054 (99%)	1006 (97%)	34 (3%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	521	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	445/449 (99%)	435 (98%)	10 (2%)	45	35
1	B	446/449 (99%)	436 (98%)	10 (2%)	45	35
All	All	891/898 (99%)	871 (98%)	20 (2%)	45	35

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	142	LYS

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Mol	Chain	Res	Type
1	A	164	LYS
1	A	190	ARG
1	A	308	LYS
1	A	309	GLU
1	A	500	ASP
1	A	501	GLU
1	A	518	MET
1	A	521	LYS
1	B	126	GLN
1	B	142	LYS
1	B	164	LYS
1	B	190	ARG
1	B	308	LYS
1	B	309	GLU
1	B	500	ASP
1	B	501	GLU
1	B	518	MET
1	B	522	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	194	ASN
1	A	280	GLN
1	A	287	ASN
1	A	288	ASN
1	A	291	ASN
1	A	302	ASN
1	A	310	GLN
1	A	312	GLN
1	A	316	ASN
1	A	324	HIS
1	A	388	ASN
1	A	390	HIS
1	A	451	GLN
1	A	478	GLN
1	A	481	GLN
1	A	514	HIS
1	B	3	ASN
1	B	186	HIS
1	B	194	ASN

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Mol	Chain	Res	Type
1	B	280	GLN
1	B	287	ASN
1	B	291	ASN
1	B	310	GLN
1	B	312	GLN
1	B	316	ASN
1	B	388	ASN
1	B	390	HIS
1	B	437	ASN
1	B	451	GLN
1	B	478	GLN
1	B	481	GLN
1	B	514	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 12 are monoatomic - leaving 76 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PE5	B	536	-	5,5,26	0.56	0	4,4,25	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PE5	B	553	-	6,6,26	0.57	0	5,5,25	0.12	0
3	EDO	B	569	-	3,3,3	0.43	0	2,2,2	0.38	0
3	EDO	A	540	-	3,3,3	0.48	0	2,2,2	0.29	0
3	EDO	A	550	-	3,3,3	0.51	0	2,2,2	0.21	0
3	EDO	A	576	-	3,3,3	0.48	0	2,2,2	0.29	0
3	EDO	A	564	-	3,3,3	0.40	0	2,2,2	0.17	0
2	PE5	A	536	-	5,5,26	0.68	0	4,4,25	0.41	0
2	PE5	B	557	-	6,6,26	0.63	0	5,5,25	0.52	0
3	EDO	A	533	-	3,3,3	0.40	0	2,2,2	0.33	0
3	EDO	A	551	-	3,3,3	0.46	0	2,2,2	0.24	0
2	PE5	B	554	-	3,3,26	0.73	0	2,2,25	0.50	0
2	PE5	A	580	-	6,6,26	0.69	0	5,5,25	0.36	0
2	PE5	B	530	-	6,6,26	0.47	0	5,5,25	0.24	0
2	PE5	A	529	-	12,12,26	0.49	0	11,11,25	0.32	0
2	PE5	B	558	-	6,6,26	0.56	0	5,5,25	0.26	0
2	PE5	A	531	-	5,5,26	0.65	0	4,4,25	0.66	0
2	PE5	A	555	-	5,5,26	0.51	0	4,4,25	0.31	0
2	PE5	B	538	-	14,14,26	0.60	0	13,13,25	0.48	0
2	PE5	B	556	-	6,6,26	0.62	0	5,5,25	0.53	0
3	EDO	A	532	-	3,3,3	0.37	0	2,2,2	0.32	0
3	EDO	A	565	-	3,3,3	0.54	0	2,2,2	0.09	0
3	EDO	B	537	-	3,3,3	0.39	0	2,2,2	0.30	0
3	EDO	B	541	-	3,3,3	0.44	0	2,2,2	0.27	0
2	PE5	A	554	-	3,3,26	0.73	0	2,2,25	0.42	0
3	EDO	B	551	-	3,3,3	0.44	0	2,2,2	0.18	0
2	PE5	A	558	-	6,6,26	0.57	0	5,5,25	0.40	0
2	PE5	B	531	-	5,5,26	0.68	0	4,4,25	0.46	0
3	EDO	B	573	-	3,3,3	0.41	0	2,2,2	0.34	0
3	EDO	A	579	-	3,3,3	0.64	0	2,2,2	0.34	0
3	EDO	B	576	-	3,3,3	0.44	0	2,2,2	0.39	0
3	EDO	B	533	-	3,3,3	0.39	0	2,2,2	0.41	0
3	EDO	A	548	-	3,3,3	0.45	0	2,2,2	0.20	0
3	EDO	B	540	-	3,3,3	0.48	0	2,2,2	0.18	0
2	PE5	B	529	-	12,12,26	0.51	0	11,11,25	0.20	0
3	EDO	A	545	-	3,3,3	0.51	0	2,2,2	0.17	0
3	EDO	A	552	-	3,3,3	0.60	0	2,2,2	0.14	0
3	EDO	A	561	-	3,3,3	0.34	0	2,2,2	0.57	0
3	EDO	B	550	-	3,3,3	0.51	0	2,2,2	0.16	0
3	EDO	B	579	-	3,3,3	0.50	0	2,2,2	0.15	0
7	PO4	A	1527	6,5	4,4,4	0.98	0	6,6,6	1.99	2 (33%)
3	EDO	A	566	-	3,3,3	0.39	0	2,2,2	0.34	0
3	EDO	A	560	-	3,3,3	0.43	0	2,2,2	0.51	0
2	PE5	B	555	-	5,5,26	0.50	0	4,4,25	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PE5	B	581	-	6,6,26	0.56	0	5,5,25	0.45	0
3	EDO	A	549	-	3,3,3	0.40	0	2,2,2	0.37	0
3	EDO	A	535[A]	-	3,3,3	0.41	0	2,2,2	0.28	0
3	EDO	B	535	-	3,3,3	0.53	0	2,2,2	0.14	0
3	EDO	B	552	-	3,3,3	0.48	0	2,2,2	0.46	0
2	PE5	A	581	-	6,6,26	0.48	0	5,5,25	0.29	0
3	EDO	A	535[B]	-	3,3,3	0.49	0	2,2,2	0.24	0
3	EDO	B	532	-	3,3,3	0.45	0	2,2,2	0.25	0
3	EDO	B	562	-	3,3,3	0.42	0	2,2,2	0.43	0
3	EDO	B	545	-	3,3,3	0.38	0	2,2,2	0.38	0
2	PE5	A	546	-	7,7,26	0.65	0	6,6,25	0.44	0
2	PE5	A	557	-	6,6,26	0.65	0	5,5,25	0.37	0
2	PE5	B	568	-	7,7,26	0.51	0	6,6,25	0.29	0
3	EDO	A	537	-	3,3,3	0.36	0	2,2,2	0.20	0
3	EDO	B	565	-	3,3,3	0.67	0	2,2,2	0.28	0
3	EDO	A	562	-	3,3,3	0.46	0	2,2,2	0.12	0
3	EDO	A	569	-	3,3,3	0.40	0	2,2,2	0.34	0
7	PO4	B	1527	6,5	4,4,4	0.79	0	6,6,6	2.10	2 (33%)
3	EDO	B	560	-	3,3,3	0.36	0	2,2,2	0.45	0
3	EDO	B	549	-	3,3,3	0.41	0	2,2,2	0.32	0
3	EDO	B	548	-	3,3,3	0.42	0	2,2,2	0.39	0
3	EDO	B	561	-	3,3,3	0.37	0	2,2,2	0.35	0
2	PE5	B	534	-	15,15,26	0.50	0	14,14,25	0.70	0
2	PE5	A	530	-	6,6,26	0.43	0	5,5,25	0.57	0
2	PE5	A	553	-	6,6,26	0.57	0	5,5,25	0.42	0
2	PE5	B	580	-	6,6,26	0.74	0	5,5,25	0.82	0
3	EDO	A	541	-	3,3,3	0.48	0	2,2,2	0.28	0
2	PE5	A	534	-	15,15,26	0.50	0	14,14,25	0.51	0
3	EDO	B	566	-	3,3,3	0.39	0	2,2,2	0.46	0
2	PE5	B	546	-	7,7,26	0.72	0	6,6,25	0.95	0
2	PE5	A	575	-	11,11,26	0.61	0	10,10,25	0.41	0
3	EDO	A	539	-	3,3,3	0.34	0	2,2,2	0.17	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	PE5	B	536	-	-	0/3/3/24	-
2	PE5	B	553	-	-	2/4/4/24	-
3	EDO	B	569	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	540	-	-	0/1/1/1	-
3	EDO	A	550	-	-	0/1/1/1	-
3	EDO	A	576	-	-	1/1/1/1	-
3	EDO	A	564	-	-	1/1/1/1	-
2	PE5	A	536	-	-	2/3/3/24	-
2	PE5	B	557	-	-	3/4/4/24	-
3	EDO	A	533	-	-	1/1/1/1	-
3	EDO	A	551	-	-	0/1/1/1	-
2	PE5	B	554	-	-	0/0/1/24	-
2	PE5	A	580	-	-	2/4/4/24	-
2	PE5	B	530	-	-	1/4/4/24	-
2	PE5	A	529	-	-	6/10/10/24	-
2	PE5	B	558	-	-	3/4/4/24	-
2	PE5	A	531	-	-	3/3/3/24	-
2	PE5	A	555	-	-	0/3/3/24	-
2	PE5	B	538	-	-	10/12/12/24	-
2	PE5	B	556	-	-	4/4/4/24	-
3	EDO	A	532	-	-	0/1/1/1	-
3	EDO	A	565	-	-	1/1/1/1	-
3	EDO	B	537	-	-	1/1/1/1	-
3	EDO	B	541	-	-	1/1/1/1	-
2	PE5	A	554	-	-	0/0/1/24	-
3	EDO	B	551	-	-	1/1/1/1	-
2	PE5	A	558	-	-	2/4/4/24	-
2	PE5	B	531	-	-	1/3/3/24	-
3	EDO	B	573	-	-	1/1/1/1	-
3	EDO	A	579	-	-	1/1/1/1	-
3	EDO	B	576	-	-	1/1/1/1	-
3	EDO	B	533	-	-	1/1/1/1	-
3	EDO	A	548	-	-	1/1/1/1	-
3	EDO	B	540	-	-	0/1/1/1	-
2	PE5	B	529	-	-	2/10/10/24	-
3	EDO	A	545	-	-	1/1/1/1	-
3	EDO	A	552	-	-	1/1/1/1	-
3	EDO	A	561	-	-	1/1/1/1	-
3	EDO	B	550	-	-	1/1/1/1	-
3	EDO	B	579	-	-	0/1/1/1	-
3	EDO	A	566	-	-	1/1/1/1	-
3	EDO	A	560	-	-	1/1/1/1	-
2	PE5	B	555	-	-	0/3/3/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PE5	B	581	-	-	1/4/4/24	-
3	EDO	A	549	-	-	1/1/1/1	-
3	EDO	A	535[A]	-	-	1/1/1/1	-
3	EDO	B	535	-	-	0/1/1/1	-
3	EDO	B	552	-	-	1/1/1/1	-
2	PE5	A	581	-	-	1/4/4/24	-
3	EDO	A	535[B]	-	-	0/1/1/1	-
3	EDO	B	532	-	-	1/1/1/1	-
3	EDO	B	562	-	-	0/1/1/1	-
3	EDO	B	545	-	-	1/1/1/1	-
2	PE5	A	546	-	-	2/5/5/24	-
2	PE5	A	557	-	-	2/4/4/24	-
2	PE5	B	568	-	-	2/5/5/24	-
3	EDO	A	537	-	-	1/1/1/1	-
3	EDO	B	565	-	-	1/1/1/1	-
3	EDO	A	562	-	-	1/1/1/1	-
3	EDO	A	569	-	-	1/1/1/1	-
3	EDO	B	560	-	-	1/1/1/1	-
3	EDO	B	549	-	-	1/1/1/1	-
3	EDO	B	548	-	-	0/1/1/1	-
3	EDO	B	561	-	-	1/1/1/1	-
2	PE5	B	534	-	-	7/13/13/24	-
2	PE5	A	530	-	-	1/4/4/24	-
2	PE5	A	553	-	-	1/4/4/24	-
2	PE5	B	580	-	-	4/4/4/24	-
3	EDO	A	541	-	-	1/1/1/1	-
2	PE5	A	534	-	-	8/13/13/24	-
3	EDO	B	566	-	-	1/1/1/1	-
2	PE5	B	546	-	-	4/5/5/24	-
2	PE5	A	575	-	-	5/9/9/24	-
3	EDO	A	539	-	-	1/1/1/1	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1527	PO4	O4-P-O2	-3.99	95.49	107.91
7	A	1527	PO4	O4-P-O2	-3.62	96.66	107.91
7	A	1527	PO4	O3-P-O2	2.64	116.13	107.91
7	B	1527	PO4	O3-P-O2	2.62	116.05	107.91

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	529	PE5	O2-C3-C4-O3
2	B	538	PE5	O2-C3-C4-O3
2	B	553	PE5	O1-C1-C2-O2
2	A	546	PE5	O1-C1-C2-O2
2	B	580	PE5	O1-C1-C2-O2
2	B	581	PE5	O1-C1-C2-O2
2	A	575	PE5	O3-C5-C6-O4
2	A	575	PE5	O2-C3-C4-O3
2	A	529	PE5	O3-C5-C6-O4
2	B	538	PE5	O3-C5-C6-O4
2	A	534	PE5	O2-C3-C4-O3
2	A	530	PE5	O1-C1-C2-O2
2	A	534	PE5	O4-C7-C8-O5
2	A	529	PE5	O4-C7-C8-O5
2	B	538	PE5	O4-C7-C8-O5
2	B	546	PE5	O2-C3-C4-O3
2	B	530	PE5	O1-C1-C2-O2
2	A	536	PE5	C48-C50-O1-C1
2	B	529	PE5	O3-C5-C6-O4
2	A	529	PE5	O1-C1-C2-O2
2	A	536	PE5	O1-C1-C2-O2
2	A	580	PE5	O1-C1-C2-O2
2	B	534	PE5	O1-C1-C2-O2
3	A	535[A]	EDO	O1-C1-C2-O2
3	A	541	EDO	O1-C1-C2-O2
3	A	552	EDO	O1-C1-C2-O2
3	A	560	EDO	O1-C1-C2-O2
3	A	562	EDO	O1-C1-C2-O2
3	A	579	EDO	O1-C1-C2-O2
3	B	532	EDO	O1-C1-C2-O2
3	B	537	EDO	O1-C1-C2-O2
3	B	550	EDO	O1-C1-C2-O2
2	A	534	PE5	O3-C5-C6-O4
2	A	531	PE5	O1-C1-C2-O2
2	B	546	PE5	C4-C3-O2-C2
2	B	568	PE5	O1-C1-C2-O2
3	A	549	EDO	O1-C1-C2-O2
3	A	564	EDO	O1-C1-C2-O2
3	A	565	EDO	O1-C1-C2-O2
3	B	545	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	573	EDO	O1-C1-C2-O2
3	B	576	EDO	O1-C1-C2-O2
2	B	558	PE5	C4-C3-O2-C2
2	A	531	PE5	C48-C50-O1-C1
2	B	546	PE5	O1-C1-C2-O2
2	B	556	PE5	O1-C1-C2-O2
2	B	558	PE5	O1-C1-C2-O2
2	B	556	PE5	C4-C3-O2-C2
2	A	557	PE5	O1-C1-C2-O2
2	B	580	PE5	C4-C3-O2-C2
3	B	541	EDO	O1-C1-C2-O2
3	B	565	EDO	O1-C1-C2-O2
3	B	566	EDO	O1-C1-C2-O2
2	B	534	PE5	C7-C8-O5-C9
2	B	557	PE5	C4-C3-O2-C2
2	A	575	PE5	C5-C6-O4-C7
2	A	546	PE5	O2-C3-C4-O3
2	B	538	PE5	C3-C4-O3-C5
2	B	529	PE5	C1-C2-O2-C3
2	A	529	PE5	C5-C6-O4-C7
2	B	538	PE5	C4-C3-O2-C2
2	B	557	PE5	C1-C2-O2-C3
2	A	529	PE5	C3-C4-O3-C5
2	A	575	PE5	O1-C1-C2-O2
2	B	534	PE5	O3-C5-C6-O4
2	B	546	PE5	C1-C2-O2-C3
2	A	534	PE5	C3-C4-O3-C5
2	B	568	PE5	O2-C3-C4-O3
2	B	556	PE5	C1-C2-O2-C3
2	B	553	PE5	C4-C3-O2-C2
2	B	538	PE5	C2-C1-O1-C50
3	B	533	EDO	O1-C1-C2-O2
3	B	569	EDO	O1-C1-C2-O2
2	A	581	PE5	C1-C2-O2-C3
2	B	534	PE5	O4-C7-C8-O5
2	A	534	PE5	O1-C1-C2-O2
2	B	538	PE5	C6-C5-O3-C4
2	B	580	PE5	C1-C2-O2-C3
2	B	538	PE5	C1-C2-O2-C3
2	B	556	PE5	C2-C1-O1-C50
2	A	534	PE5	C48-C50-O1-C1
3	B	549	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	552	EDO	O1-C1-C2-O2
3	B	561	EDO	O1-C1-C2-O2
2	B	531	PE5	C2-C1-O1-C50
2	A	558	PE5	C4-C3-O2-C2
2	B	538	PE5	C8-C7-O4-C6
3	A	569	EDO	O1-C1-C2-O2
2	A	580	PE5	C2-C1-O1-C50
2	B	580	PE5	C2-C1-O1-C50
2	A	575	PE5	C4-C3-O2-C2
3	A	533	EDO	O1-C1-C2-O2
3	A	539	EDO	O1-C1-C2-O2
3	A	548	EDO	O1-C1-C2-O2
3	A	566	EDO	O1-C1-C2-O2
3	A	576	EDO	O1-C1-C2-O2
2	B	534	PE5	C8-C7-O4-C6
2	A	534	PE5	C7-C8-O5-C9
2	B	534	PE5	C5-C6-O4-C7
3	A	537	EDO	O1-C1-C2-O2
3	B	551	EDO	O1-C1-C2-O2
2	B	538	PE5	C48-C50-O1-C1
2	A	557	PE5	C4-C3-O2-C2
2	A	531	PE5	C2-C1-O1-C50
3	B	560	EDO	O1-C1-C2-O2
2	A	558	PE5	O1-C1-C2-O2
2	B	534	PE5	C48-C50-O1-C1
2	B	558	PE5	C1-C2-O2-C3
2	A	553	PE5	O1-C1-C2-O2
2	B	557	PE5	O1-C1-C2-O2
2	A	534	PE5	C5-C6-O4-C7
3	A	545	EDO	O1-C1-C2-O2
3	A	561	EDO	O1-C1-C2-O2

There are no ring outliers.

27 monomers are involved in 64 short contacts:

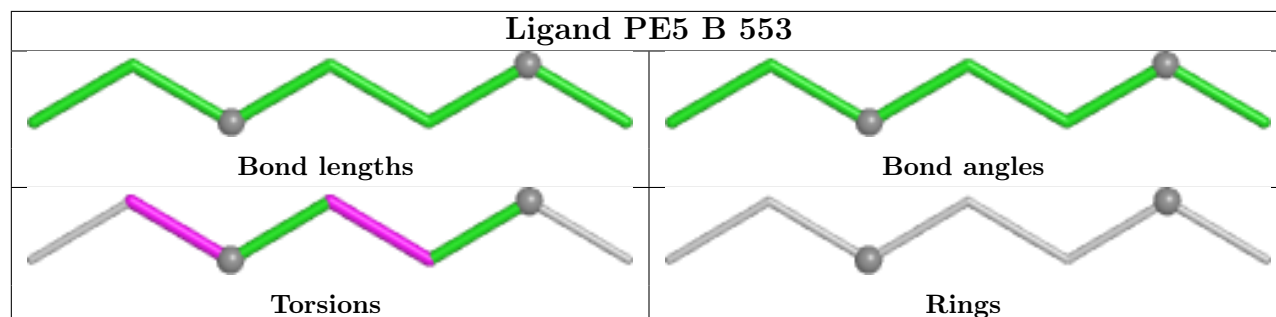
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	536	PE5	2	0
3	A	564	EDO	3	0
2	A	536	PE5	2	0
2	B	557	PE5	1	0
2	B	554	PE5	2	0
2	A	580	PE5	1	0

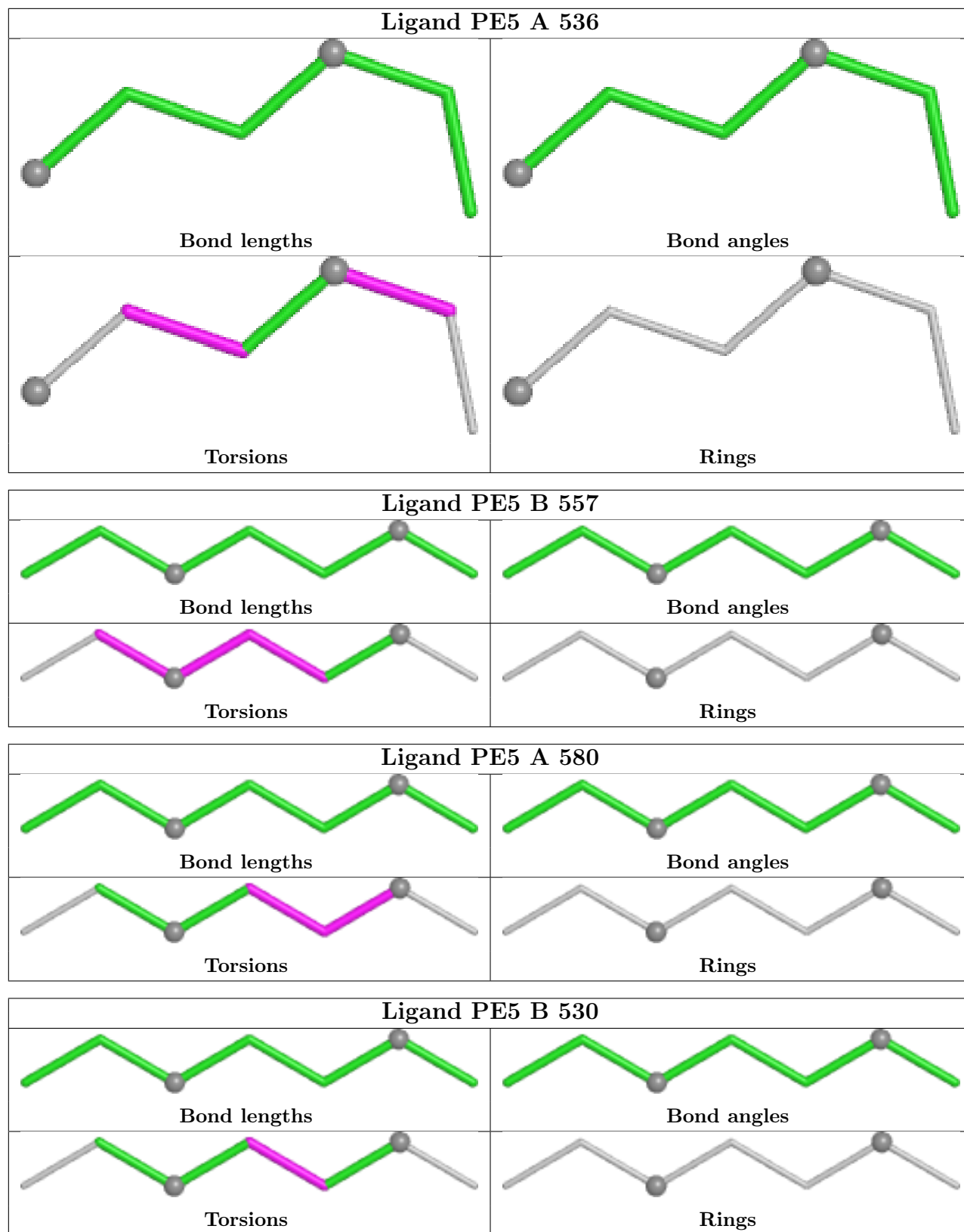
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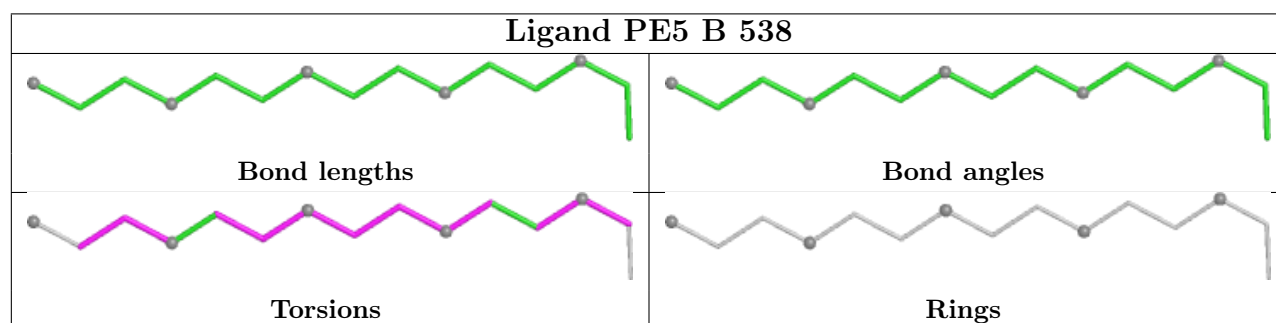
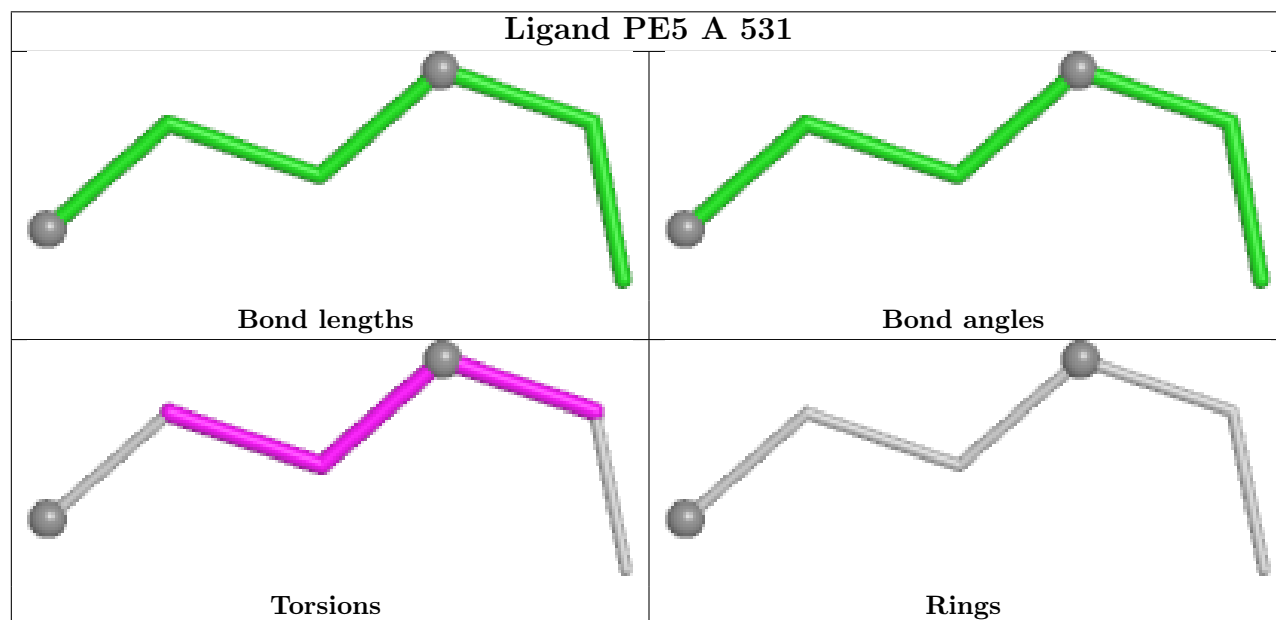
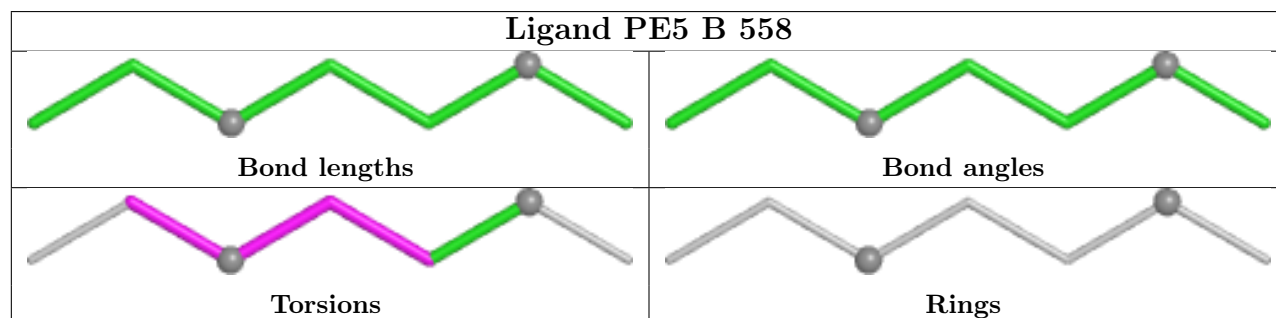
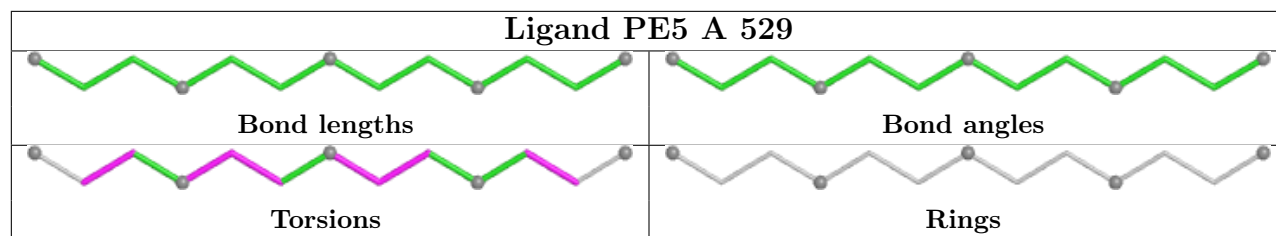
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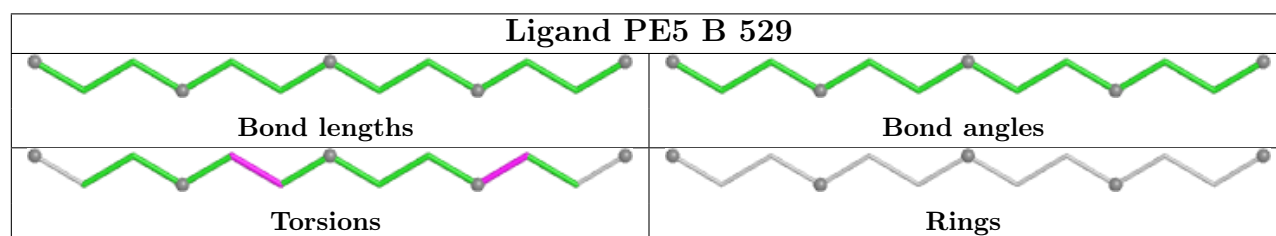
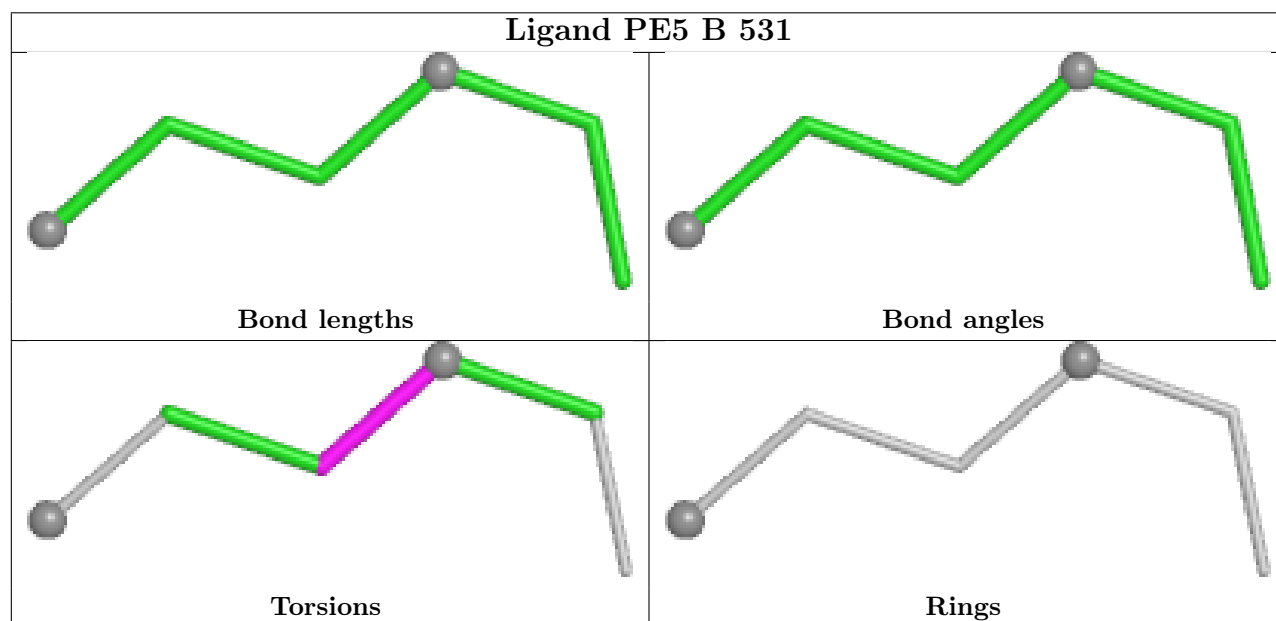
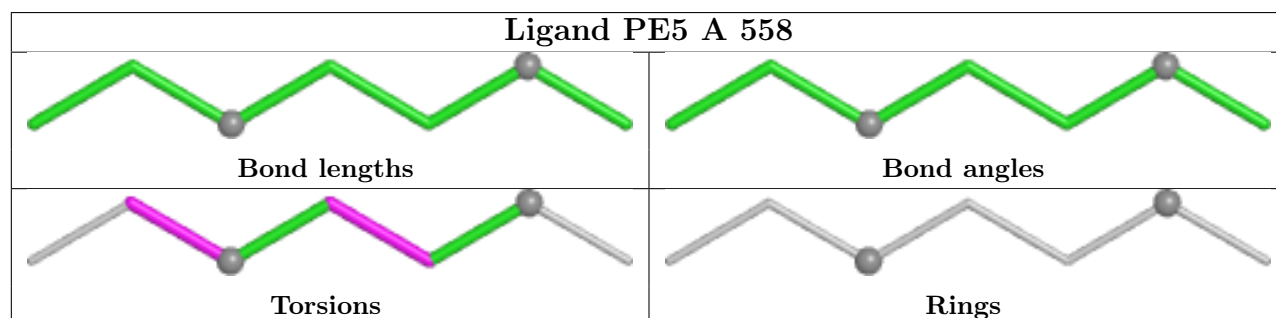
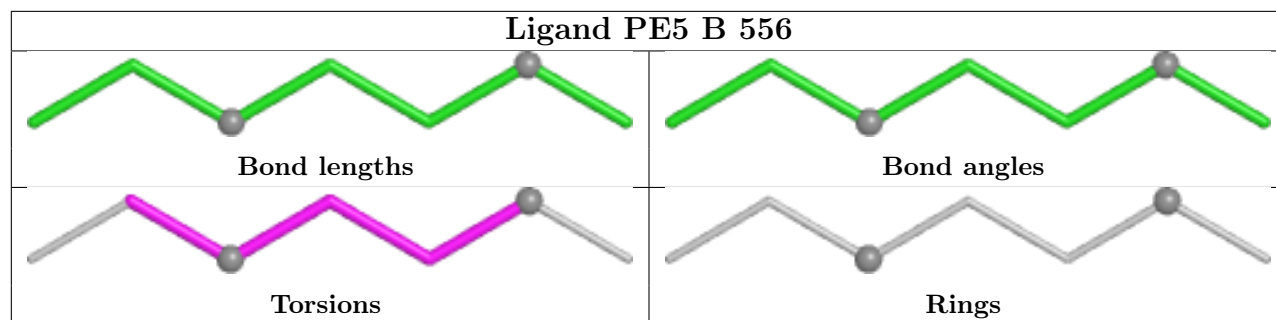
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	529	PE5	1	0
3	A	565	EDO	1	0
3	B	541	EDO	2	0
2	A	554	PE5	2	0
3	A	579	EDO	4	0
3	B	576	EDO	1	0
3	A	552	EDO	1	0
3	B	550	EDO	1	0
3	B	579	EDO	1	0
3	A	566	EDO	4	0
2	B	581	PE5	3	0
3	B	552	EDO	1	0
2	A	581	PE5	2	0
2	A	546	PE5	1	0
2	A	557	PE5	1	0
3	B	565	EDO	1	0
3	A	569	EDO	4	0
2	B	534	PE5	9	0
2	B	580	PE5	1	0
2	A	534	PE5	7	0
3	A	539	EDO	5	0

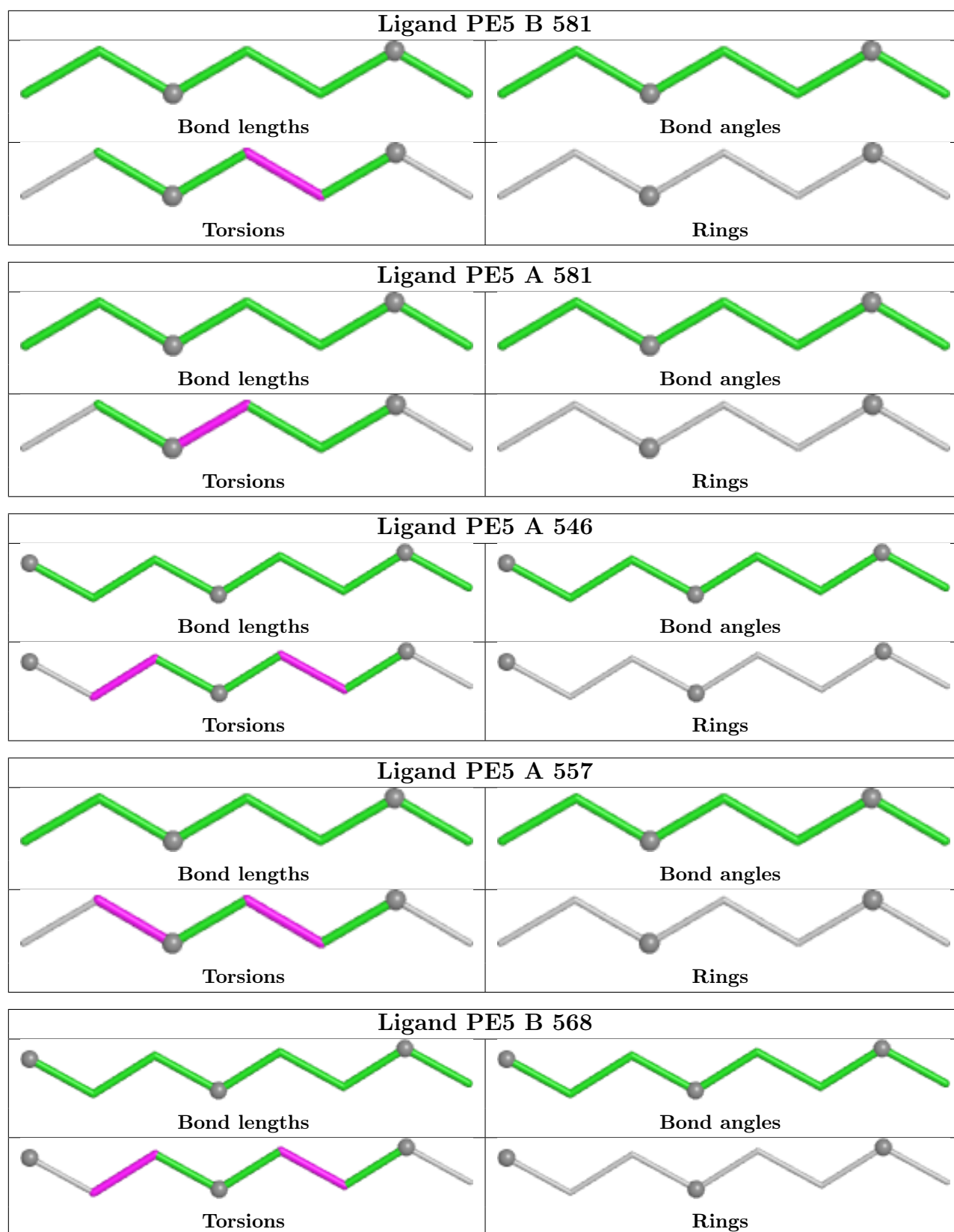
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

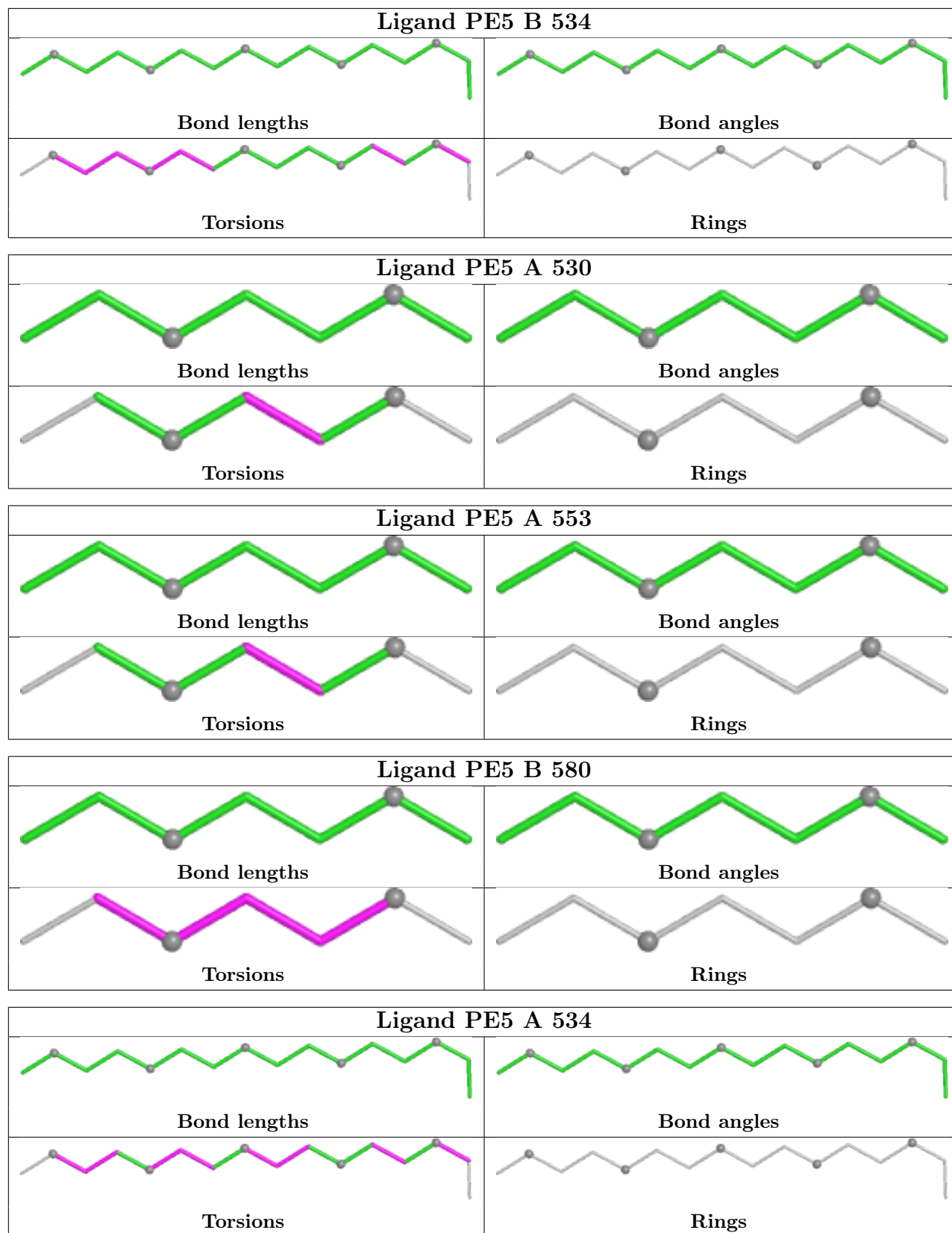


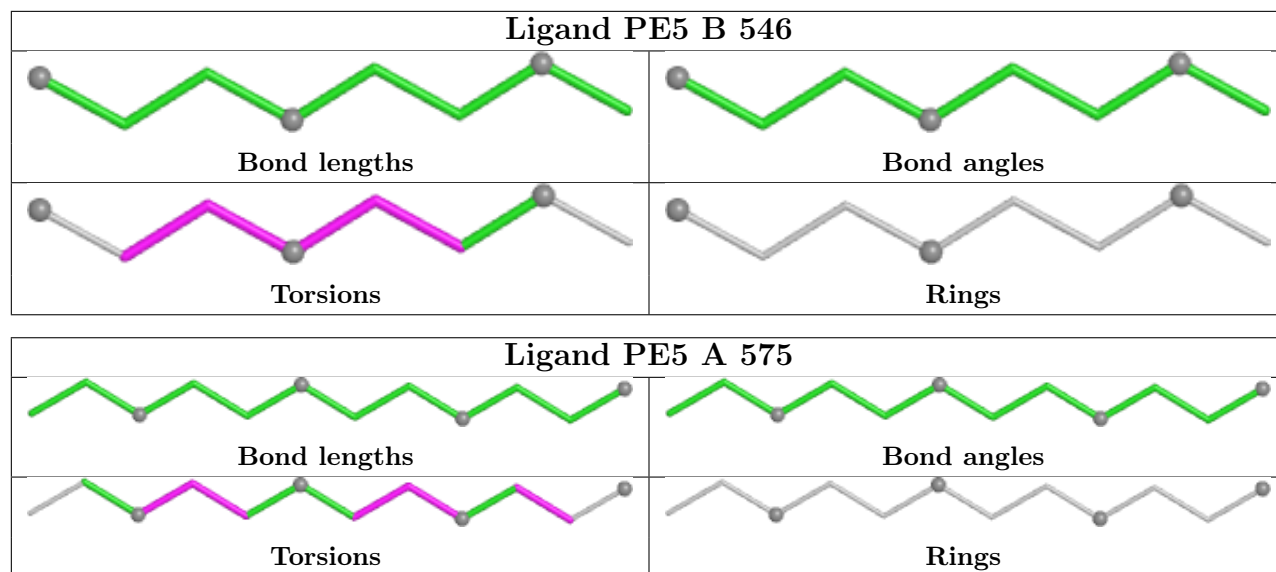












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	522/527 (99%)	-0.06	14 (2%) 56 63	15, 24, 44, 89	0
1	B	522/527 (99%)	0.21	26 (4%) 34 38	11, 27, 50, 91	1 (0%)
All	All	1044/1054 (99%)	0.07	40 (3%) 44 49	11, 25, 48, 91	1 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	6.7
1	B	1	ALA	4.6
1	B	395	LYS	4.6
1	B	522	ARG	3.9
1	A	522	ARG	3.8
1	A	501	GLU	3.7
1	B	393	PHE	3.6
1	B	518	MET	3.5
1	A	518	MET	3.4
1	B	507	PHE	3.3
1	A	113	ASN	3.3
1	B	501	GLU	3.2
1	B	391	VAL	3.2
1	A	164	LYS	2.7
1	B	394	GLU	2.7
1	B	428	LYS	2.7
1	A	519	ILE	2.6
1	A	428	LYS	2.6
1	A	509	SER	2.6
1	B	370	ASN	2.5
1	B	485	ARG	2.4
1	A	507	PHE	2.4
1	B	296	ASP	2.4
1	B	164	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	394	GLU	2.3
1	B	114	VAL	2.3
1	B	396	THR	2.3
1	B	516	LYS	2.2
1	A	515	GLU	2.2
1	B	508	PHE	2.2
1	B	425	GLN	2.1
1	B	397	SER	2.1
1	B	342	SER	2.1
1	A	511	ASN	2.1
1	B	113	ASN	2.1
1	A	296	ASP	2.1
1	B	392	ASP	2.1
1	B	514	HIS	2.0
1	B	344	SER	2.0
1	B	431	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PE5	A	536	6/27	0.69	0.29	54,57,61,76	0
2	PE5	B	536	6/27	0.72	0.28	50,51,60,61	0
2	PE5	B	553	7/27	0.72	0.29	56,60,63,65	0
2	PE5	B	554	4/27	0.72	0.36	43,58,61,65	0
2	PE5	B	580	7/27	0.72	0.31	45,55,62,63	0
2	PE5	B	556	7/27	0.75	0.24	60,66,70,71	0
2	PE5	B	555	6/27	0.75	0.26	55,61,64,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PE5	A	580	7/27	0.76	0.27	53,54,65,66	0
2	PE5	A	546	8/27	0.78	0.21	45,53,54,59	0
2	PE5	B	546	8/27	0.79	0.19	45,51,54,56	0
2	PE5	B	531	6/27	0.79	0.27	49,55,57,64	0
2	PE5	B	568	8/27	0.80	0.24	66,71,79,88	0
2	PE5	A	553	7/27	0.80	0.23	47,57,61,65	0
3	EDO	B	566	4/4	0.80	0.23	65,66,68,74	0
2	PE5	B	538	15/27	0.81	0.23	42,53,67,69	0
2	PE5	A	575	12/27	0.81	0.23	44,57,72,75	0
2	PE5	A	554	4/27	0.81	0.27	31,48,53,54	0
2	PE5	A	581	7/27	0.82	0.19	43,56,60,60	0
2	PE5	B	558	7/27	0.82	0.25	53,59,68,71	0
2	PE5	A	557	7/27	0.82	0.20	31,46,55,58	0
2	PE5	A	531	6/27	0.82	0.23	41,43,47,53	0
2	PE5	B	581	7/27	0.82	0.20	45,53,58,61	0
3	EDO	A	552	4/4	0.82	0.27	44,46,56,57	0
3	EDO	B	562	4/4	0.82	0.24	52,64,65,76	0
2	PE5	A	555	6/27	0.82	0.24	53,59,64,66	0
3	EDO	A	579	4/4	0.83	0.28	50,55,60,60	0
2	PE5	B	529	13/27	0.83	0.17	48,58,62,65	0
3	EDO	A	576	4/4	0.83	0.26	55,67,71,78	0
3	EDO	B	576	4/4	0.83	0.23	52,53,54,61	4
3	EDO	B	535	4/4	0.84	0.22	56,61,64,66	0
2	PE5	A	558	7/27	0.84	0.24	50,55,62,64	0
2	PE5	B	557	7/27	0.85	0.21	30,54,63,65	0
3	EDO	A	560	4/4	0.85	0.19	53,62,64,67	0
2	PE5	B	534	16/27	0.86	0.18	36,48,58,58	0
2	PE5	A	529	13/27	0.86	0.15	51,57,62,68	0
3	EDO	B	552	4/4	0.86	0.25	43,53,53,65	0
3	EDO	B	579	4/4	0.86	0.22	62,64,64,69	0
3	EDO	A	537	4/4	0.87	0.15	46,51,54,62	0
3	EDO	A	564	4/4	0.87	0.20	37,42,43,49	0
3	EDO	B	533	4/4	0.87	0.17	52,53,55,61	0
3	EDO	B	550	4/4	0.88	0.16	43,50,50,56	0
3	EDO	A	566	4/4	0.88	0.17	49,50,54,58	0
3	EDO	A	545	4/4	0.88	0.13	49,54,56,56	0
3	EDO	A	535[A]	4/4	0.88	0.19	32,34,35,38	4
3	EDO	A	535[B]	4/4	0.88	0.19	23,24,26,29	4
2	PE5	A	534	16/27	0.88	0.17	36,53,61,68	0
3	EDO	A	551	4/4	0.89	0.21	66,67,68,69	0
3	EDO	B	551	4/4	0.89	0.16	62,63,64,67	0
3	EDO	B	565	4/4	0.89	0.20	37,50,53,59	0

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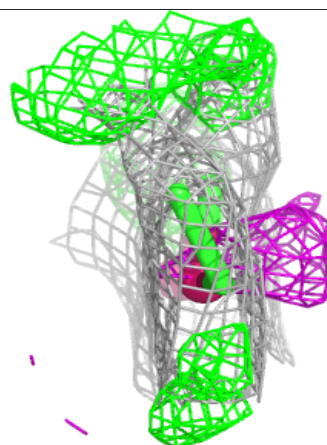
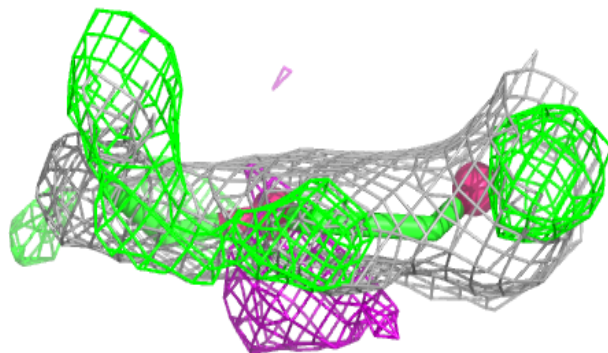
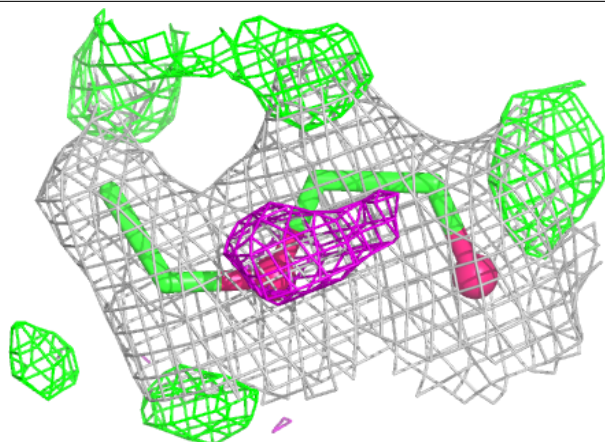
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	550	4/4	0.90	0.14	40,50,53,58	0
2	PE5	A	530	7/27	0.90	0.13	38,39,45,46	0
3	EDO	A	548	4/4	0.90	0.16	28,33,38,38	4
3	EDO	A	541	4/4	0.91	0.20	25,37,38,47	4
3	EDO	B	545	4/4	0.91	0.12	42,48,58,61	0
3	EDO	B	569	4/4	0.91	0.14	36,42,46,52	0
3	EDO	B	573	4/4	0.91	0.17	48,50,55,58	0
3	EDO	B	560	4/4	0.91	0.13	54,55,58,68	0
2	PE5	B	530	7/27	0.91	0.14	40,43,47,51	0
3	EDO	A	562	4/4	0.92	0.15	50,53,57,61	0
3	EDO	A	569	4/4	0.92	0.12	42,43,52,59	0
3	EDO	A	533	4/4	0.92	0.14	47,50,50,55	0
3	EDO	B	549	4/4	0.92	0.14	44,53,55,57	0
3	EDO	A	565	4/4	0.92	0.17	39,53,54,65	0
3	EDO	B	537	4/4	0.93	0.14	45,46,47,53	0
3	EDO	B	541	4/4	0.93	0.18	27,40,40,47	4
3	EDO	A	561	4/4	0.93	0.13	38,42,42,42	0
3	EDO	B	540	4/4	0.94	0.13	48,50,51,51	0
3	EDO	A	549	4/4	0.94	0.13	40,44,47,52	0
3	EDO	A	539	4/4	0.94	0.23	24,25,26,26	4
3	EDO	B	548	4/4	0.94	0.12	30,34,39,42	4
3	EDO	B	561	4/4	0.95	0.13	39,47,48,51	0
3	EDO	A	532	4/4	0.96	0.15	47,48,48,57	0
3	EDO	B	532	4/4	0.96	0.14	51,52,53,56	0
4	NA	A	1585	1/1	0.96	0.10	23,23,23,23	0
4	NA	B	1585	1/1	0.96	0.08	26,26,26,26	0
3	EDO	A	540	4/4	0.97	0.09	29,34,34,36	0
4	NA	B	582	1/1	0.98	0.03	16,16,16,16	0
4	NA	A	582	1/1	0.98	0.03	14,14,14,14	0
6	CA	A	1526	1/1	0.98	0.03	20,20,20,20	0
7	PO4	B	1527	5/5	0.98	0.05	20,21,21,22	0
5	FE	A	1524	1/1	0.99	0.03	17,17,17,17	0
5	FE	B	1524	1/1	0.99	0.02	19,19,19,19	0
6	CA	A	1525	1/1	0.99	0.03	18,18,18,18	0
4	NA	A	577	1/1	0.99	0.02	13,13,13,13	0
6	CA	B	1525	1/1	0.99	0.03	20,20,20,20	0
6	CA	B	1526	1/1	0.99	0.03	23,23,23,23	0
7	PO4	A	1527	5/5	0.99	0.04	16,18,19,19	0
4	NA	B	577	1/1	0.99	0.03	19,19,19,19	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.

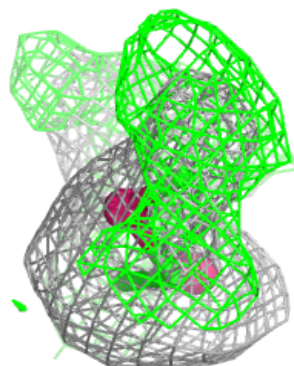
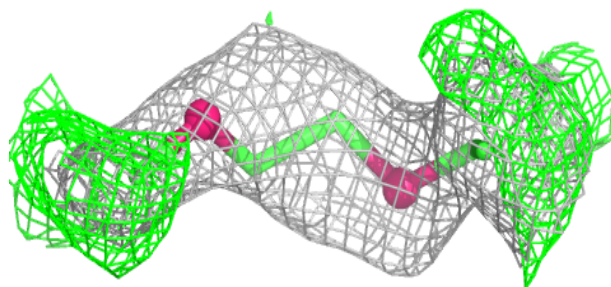
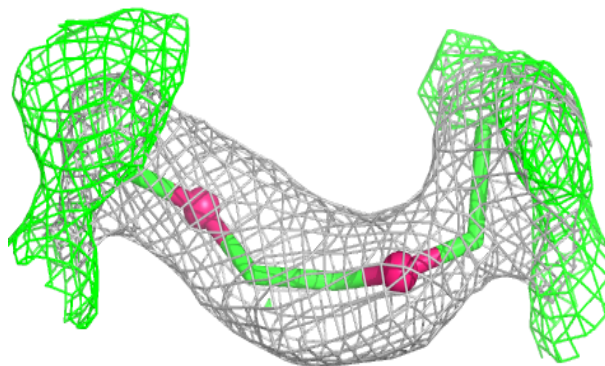
Electron density around PE5 A 536:

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

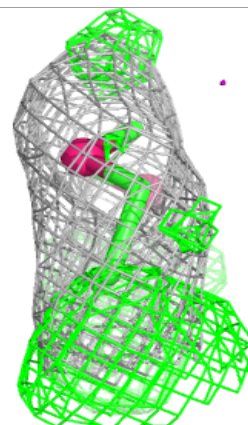
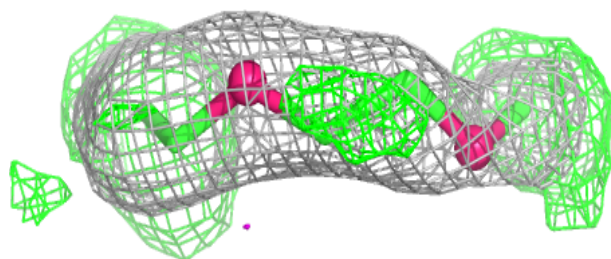
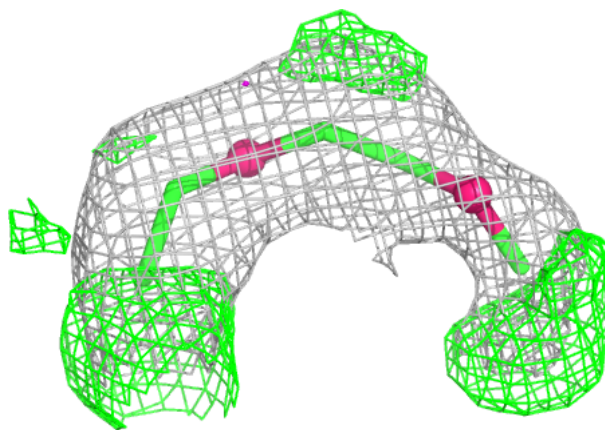


Electron density around PE5 B 553:

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

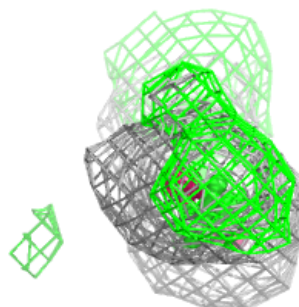
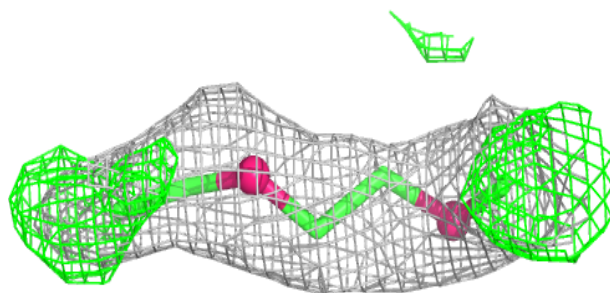
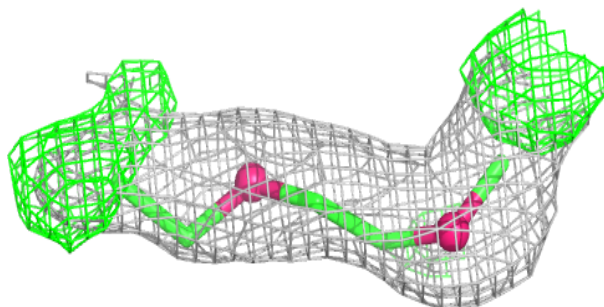
**Electron density around PE5 B 580:**

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

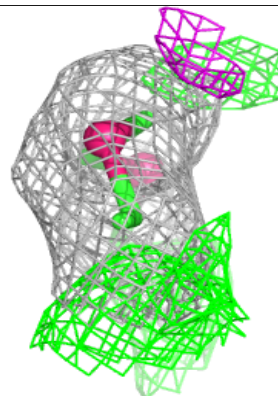
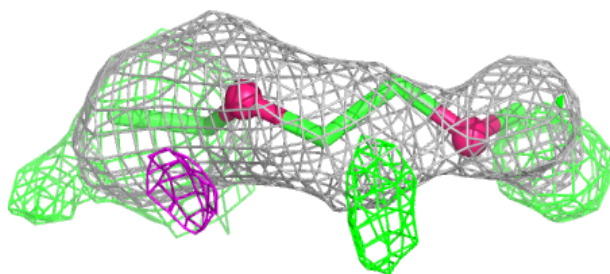
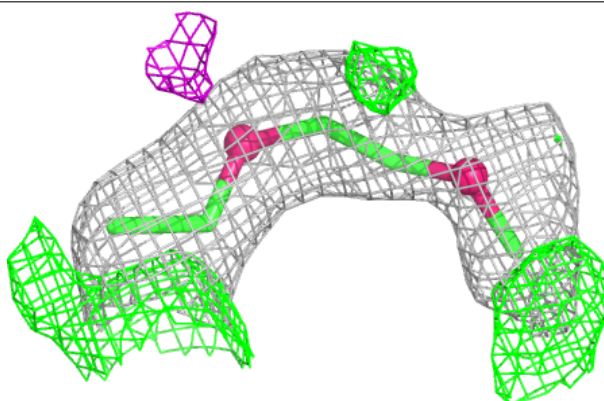


Electron density around PE5 B 556:

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

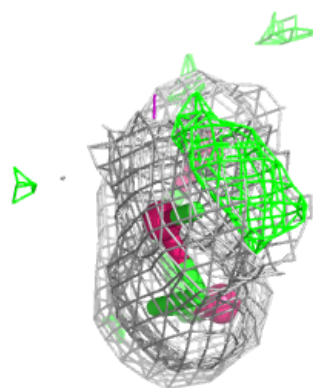
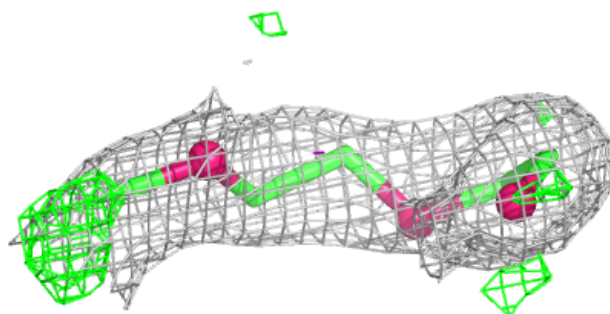
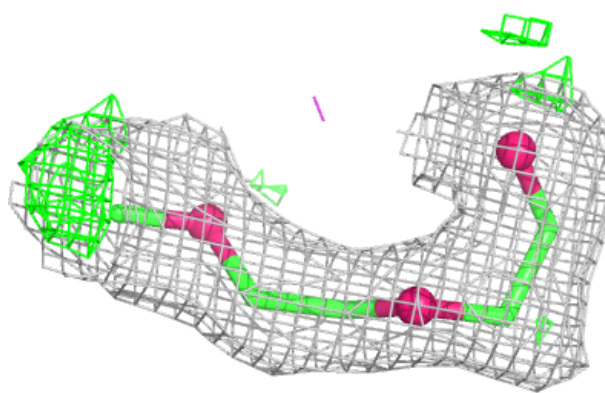
**Electron density around PE5 A 580:**

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

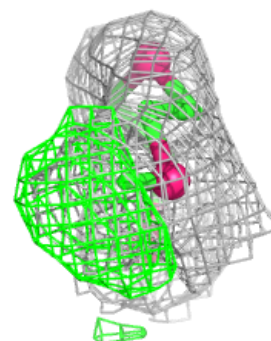
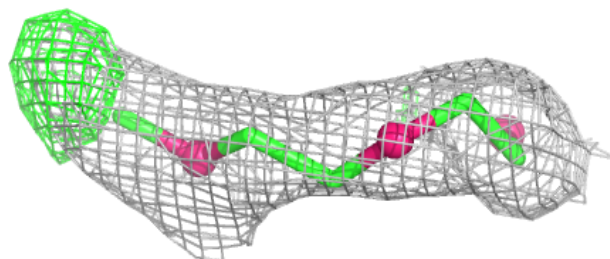
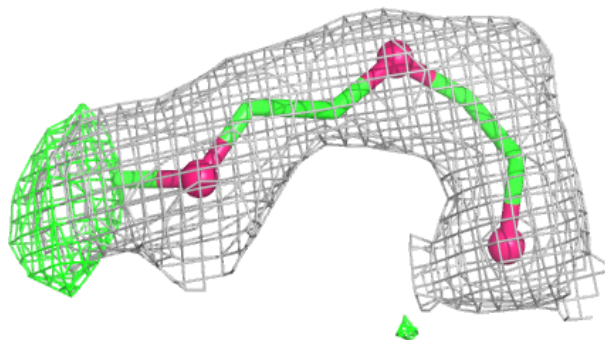


Electron density around PE5 A 546:

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

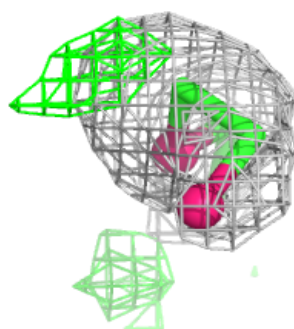
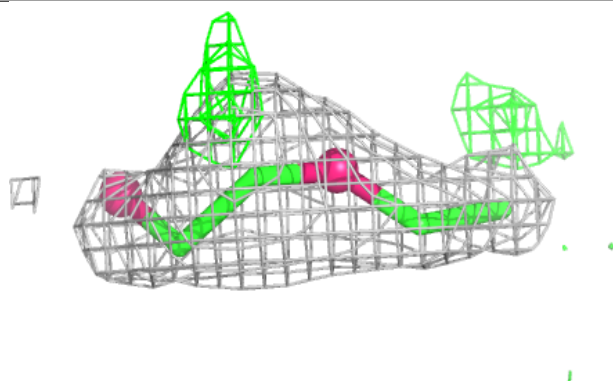
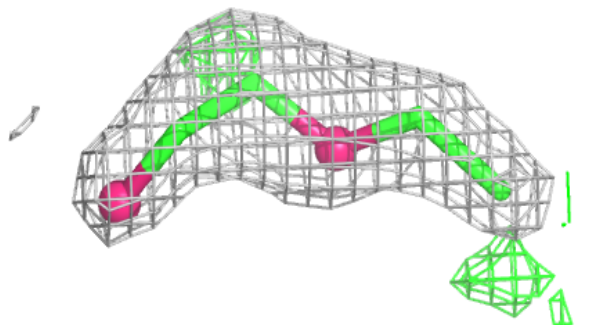
**Electron density around PE5 B 546:**

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

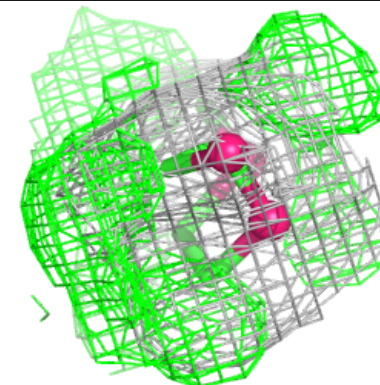
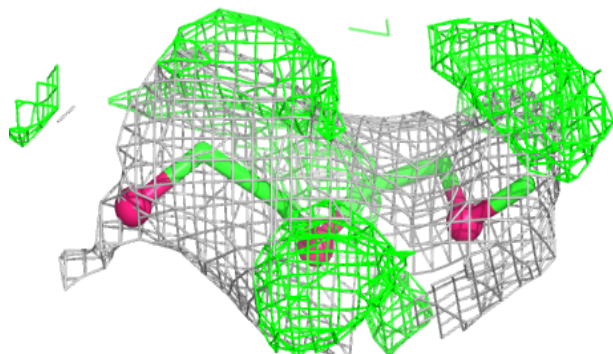
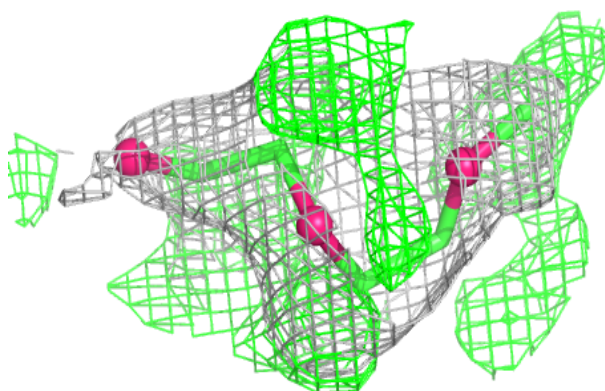


Electron density around PE5 B 531:

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

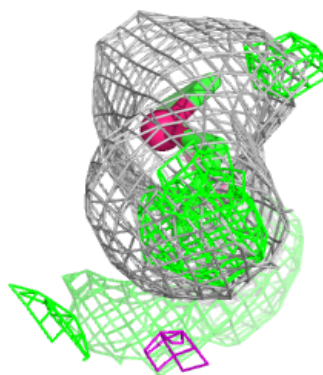
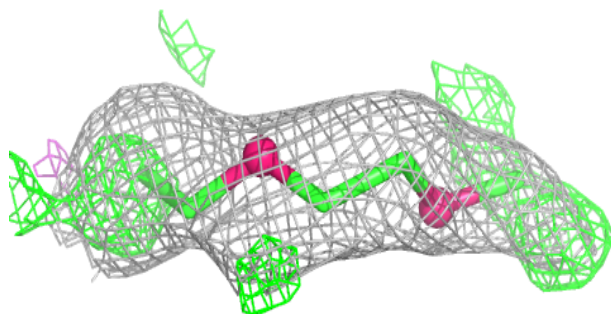
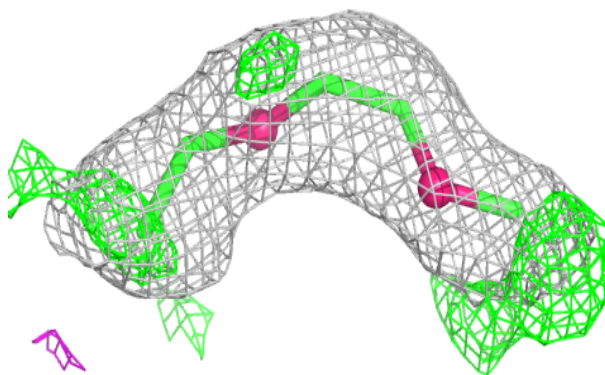
**Electron density around PE5 B 568:**

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

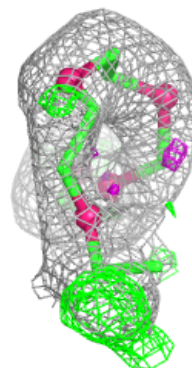
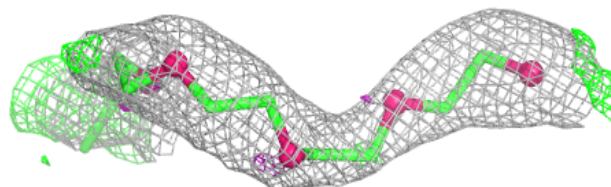
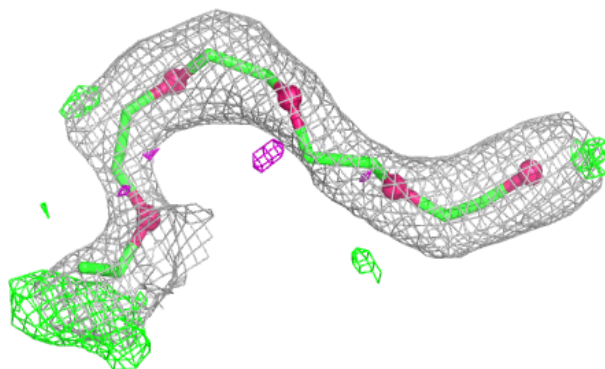


Electron density around PE5 A 553:

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

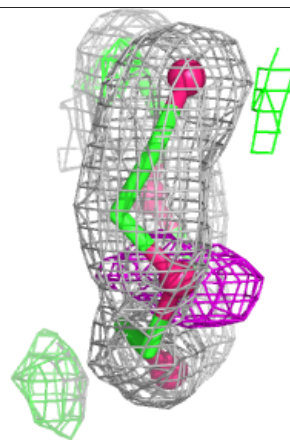
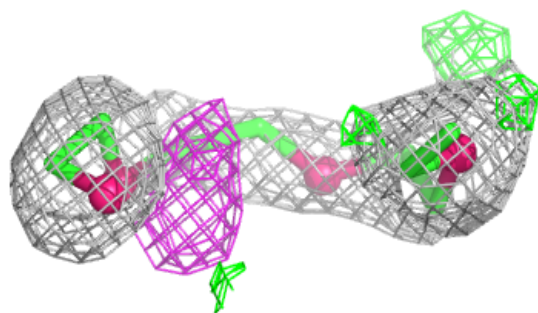
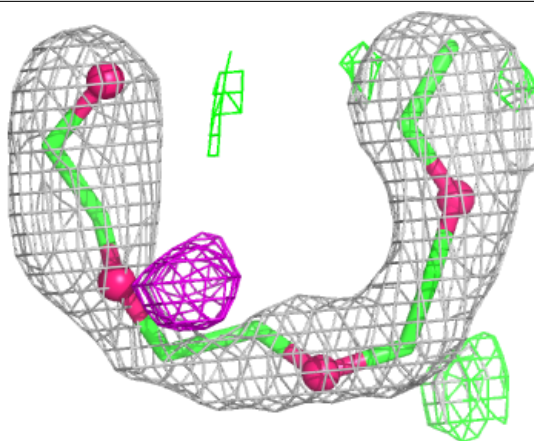
**Electron density around PE5 B 538:**

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



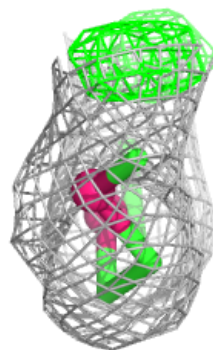
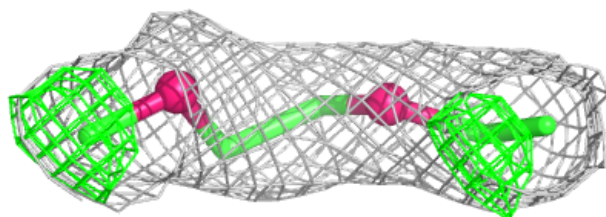
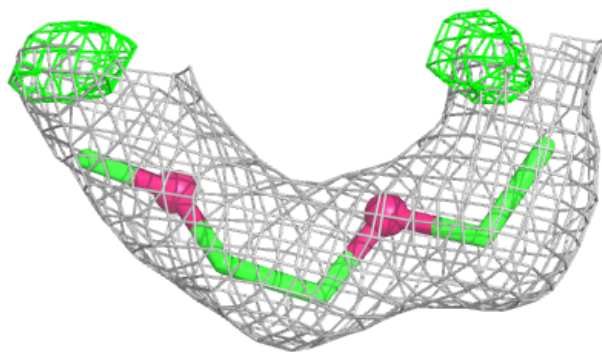
Electron density around PE5 A 575:

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



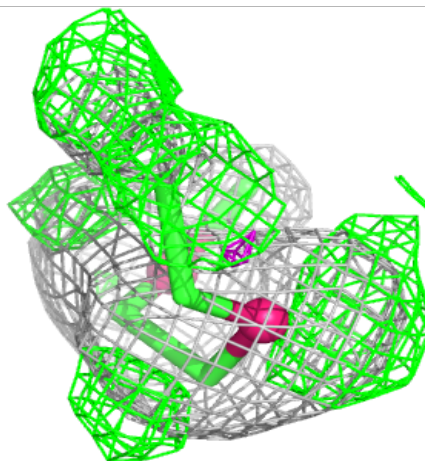
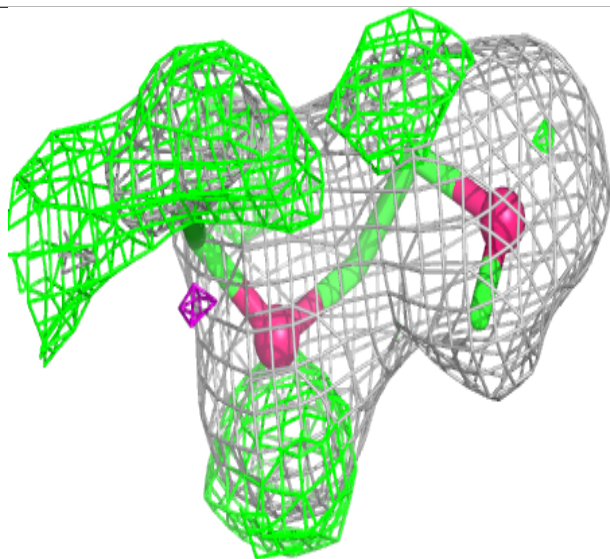
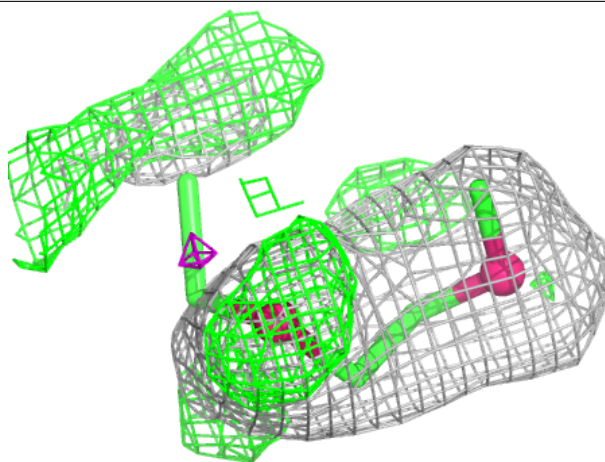
Electron density around PE5 A 581:

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



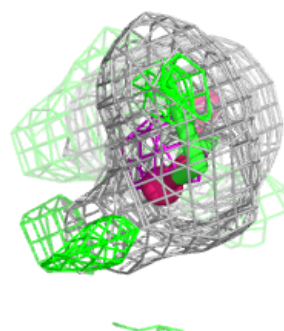
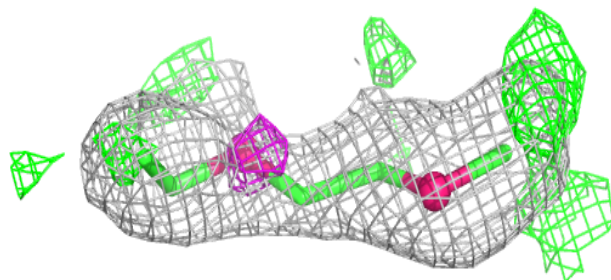
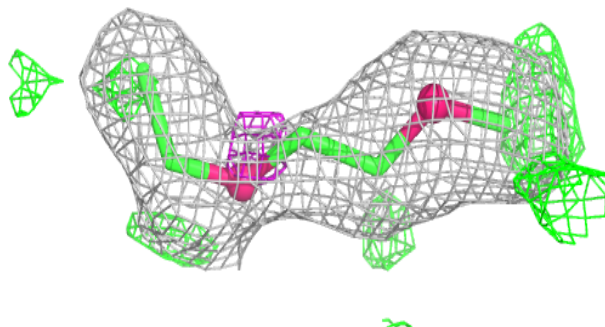
Electron density around PE5 B 558:

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

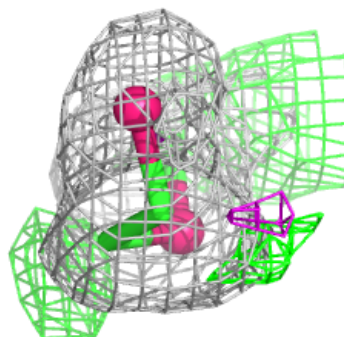
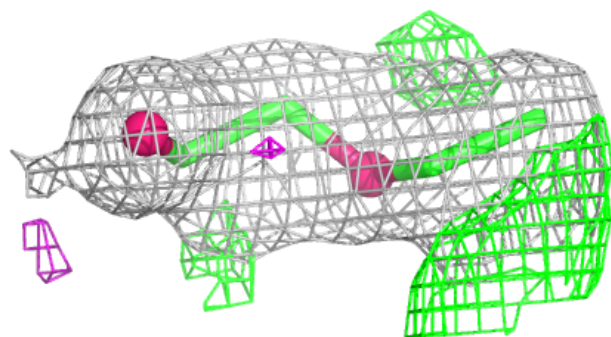
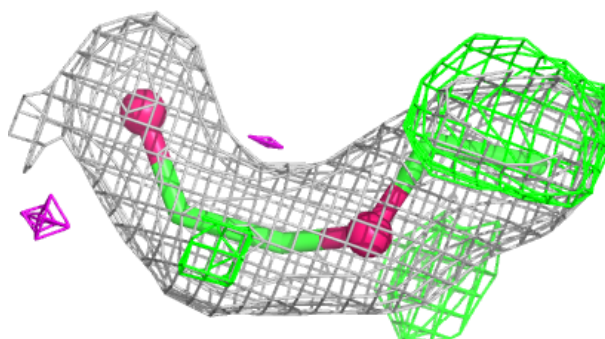


Electron density around PE5 A 557:

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

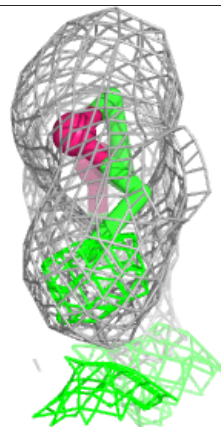
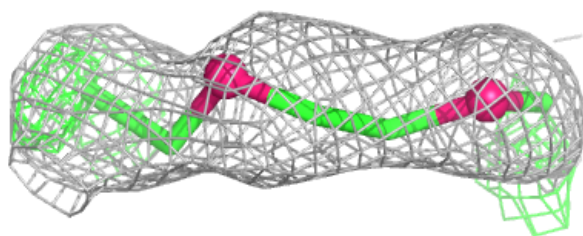
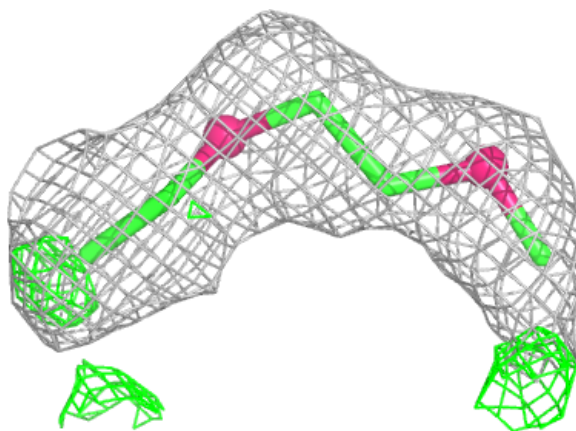
**Electron density around PE5 A 531:**

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



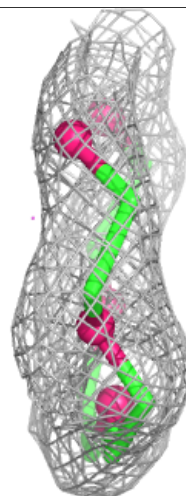
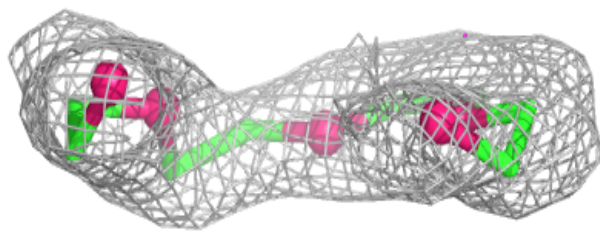
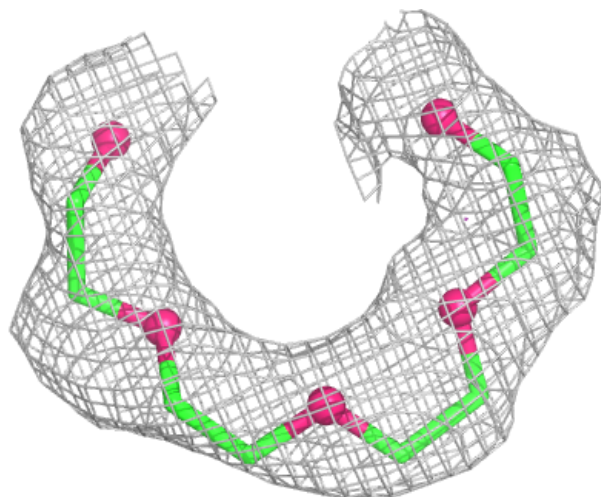
Electron density around PE5 B 581:

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



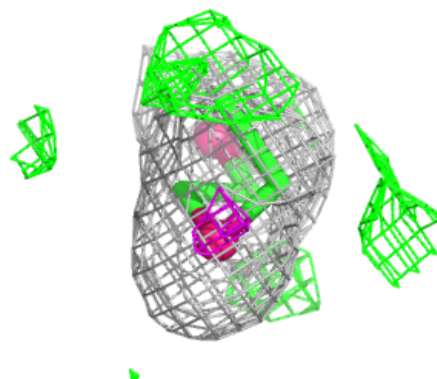
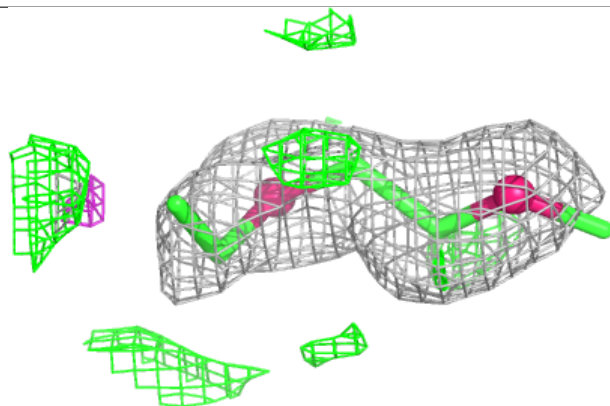
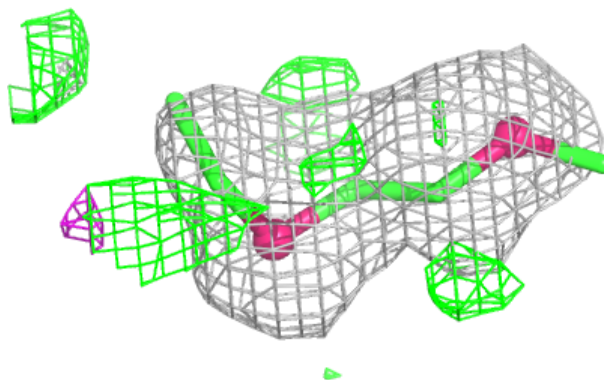
Electron density around PE5 B 529:

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

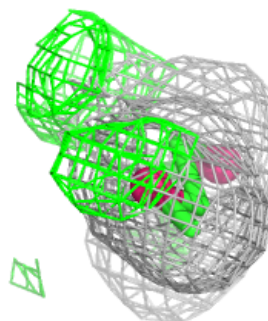
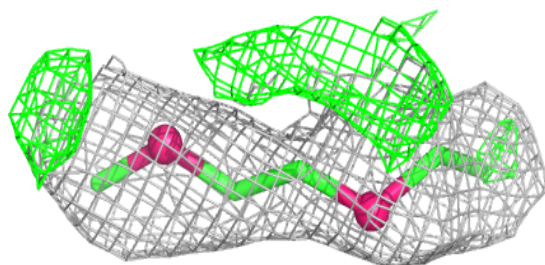
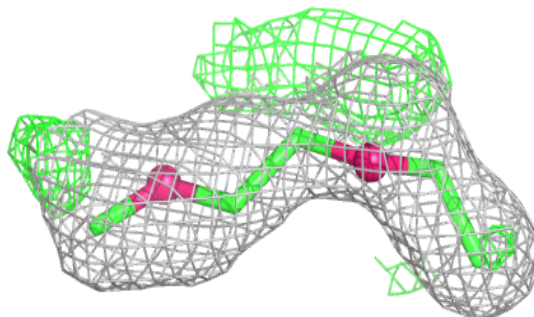


Electron density around PE5 A 558:

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

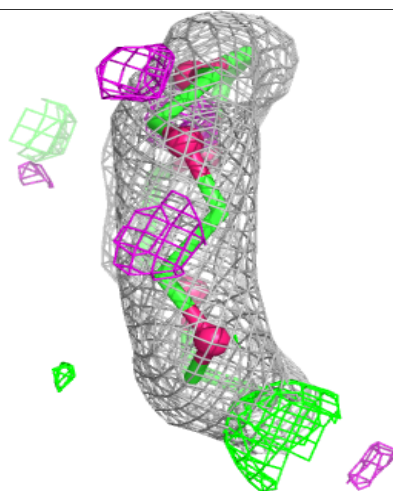
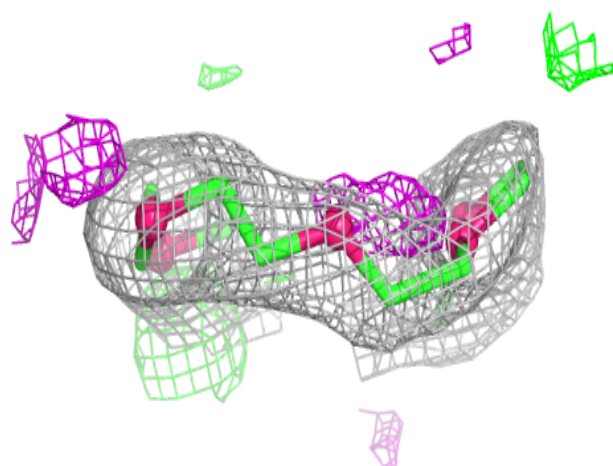
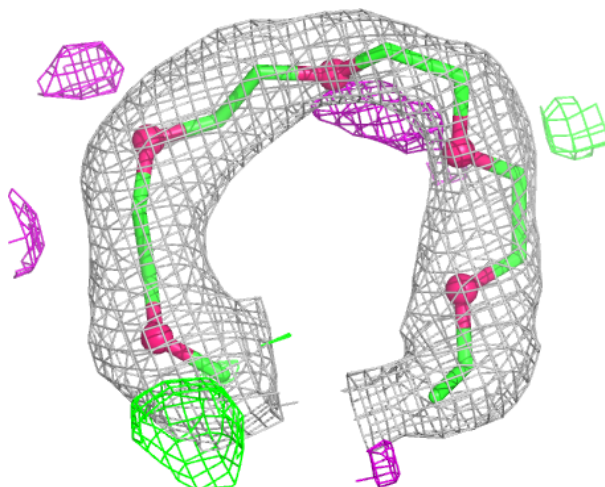
**Electron density around PE5 B 557:**

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



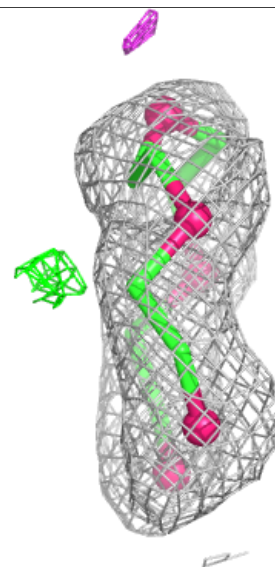
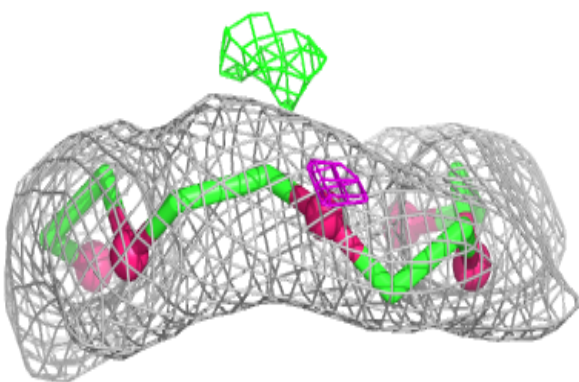
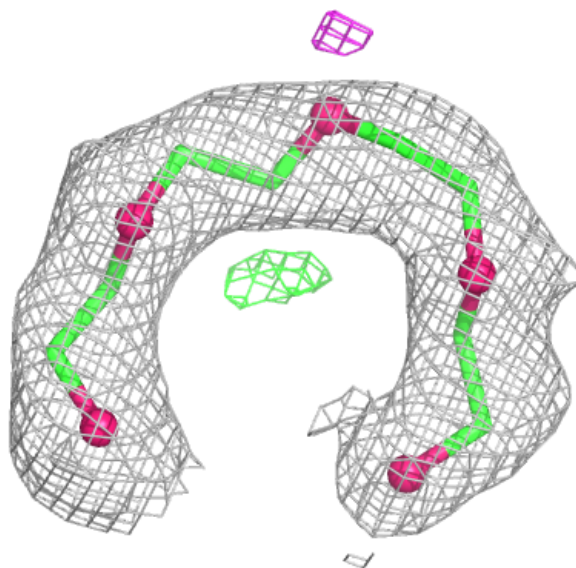
Electron density around PE5 B 534:

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



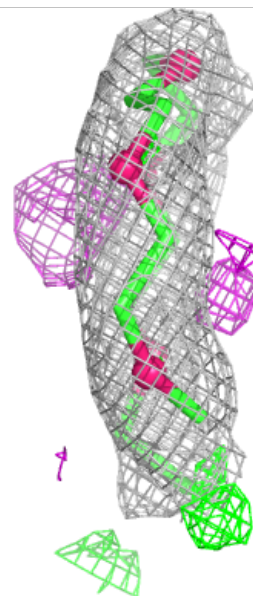
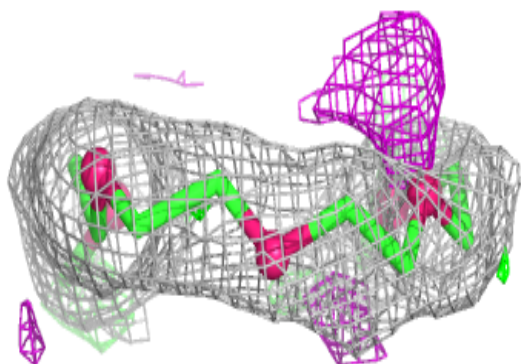
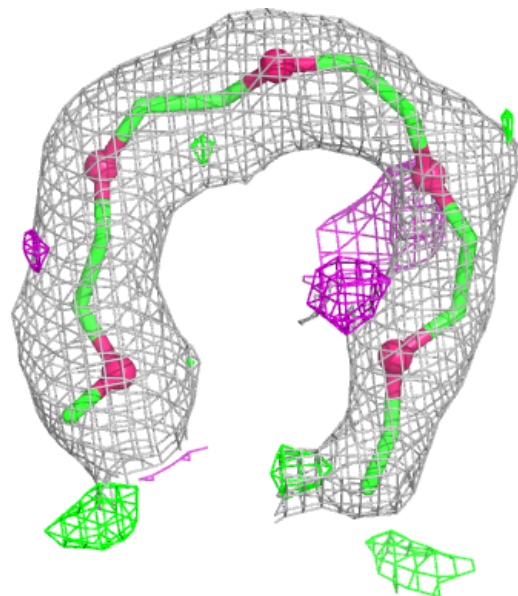
Electron density around PE5 A 529:

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



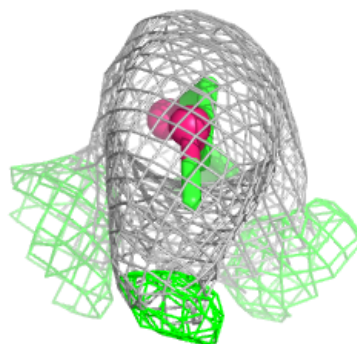
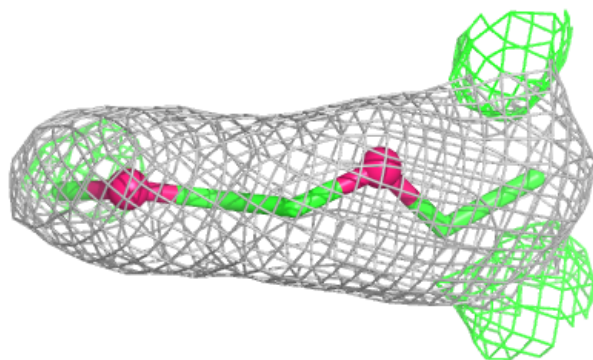
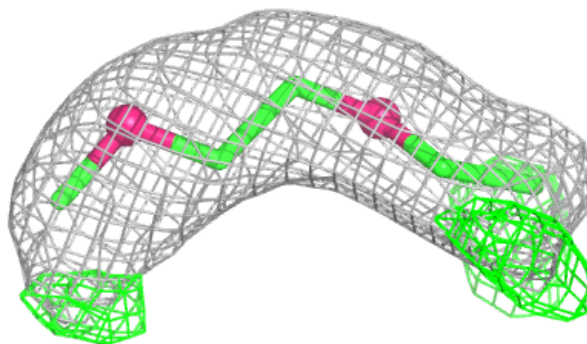
Electron density around PE5 A 534:

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

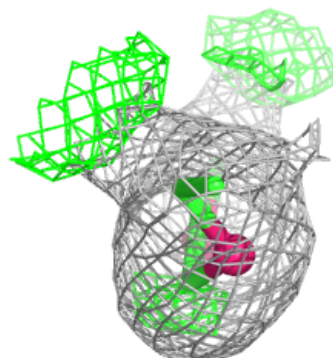
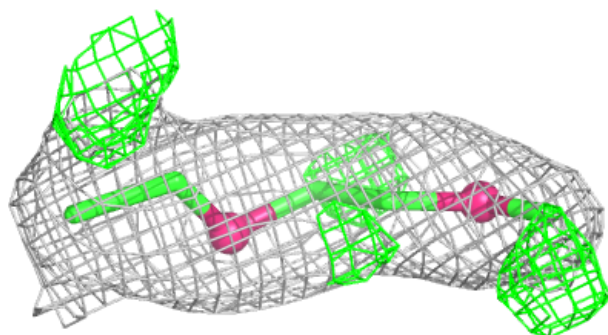
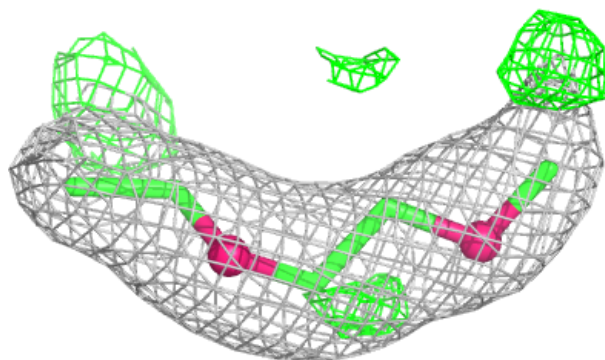


Electron density around PE5 A 530:

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

**Electron density around PE5 B 530:**

$2mF_o-DF_c$ (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.