



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 11:34 PM UTC

PDB ID : 9UAY / pdb_00009uay
Title : Crystal structure of CmnI
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Deposited on : 2025-04-01
Resolution : 2.17 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

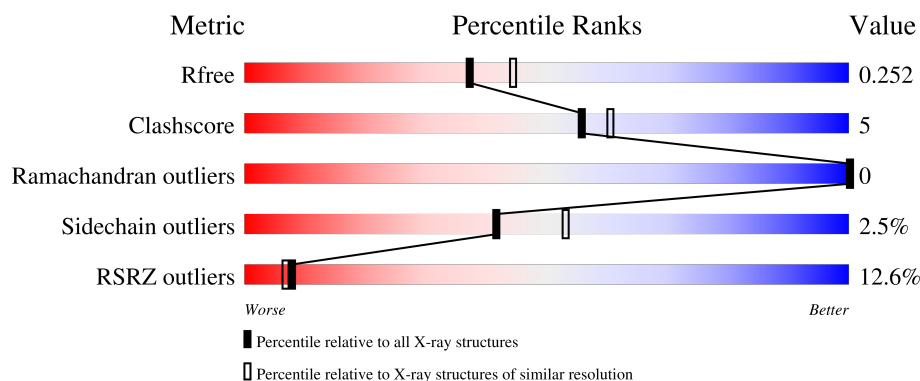
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	568	<div> <div>5%</div> <div>68%</div> <div>7%</div> <div>24%</div> </div>
1	B	568	<div> <div>14%</div> <div>64%</div> <div>10%</div> <div>26%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	AE3	B	605	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6862 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 CmnI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	1	0
			3362	2122	625	612	3			
1	B	419	Total	C	N	O	S	0	1	0
			3277	2074	602	598	3			

There are 40 discrepancies between the modelled and reference sequences:

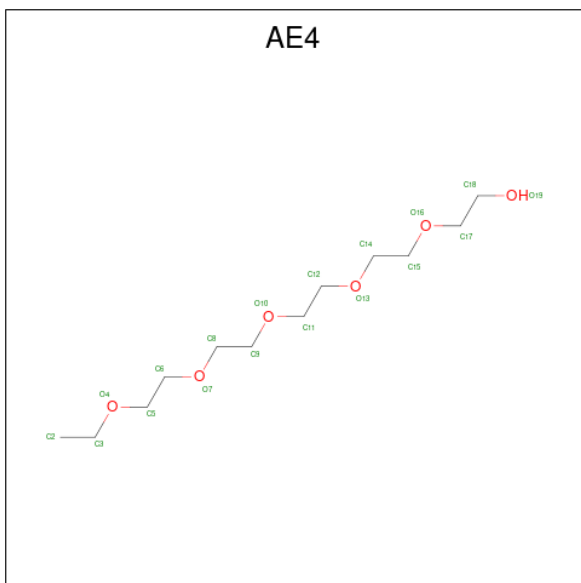
Chain	Residue	Modelled	Actual	Comment	Reference
A	-116	MET	-	initiating methionine	UNP A6YEI0
A	-115	GLY	-	expression tag	UNP A6YEI0
A	-114	SER	-	expression tag	UNP A6YEI0
A	-113	SER	-	expression tag	UNP A6YEI0
A	-112	HIS	-	expression tag	UNP A6YEI0
A	-111	HIS	-	expression tag	UNP A6YEI0
A	-110	HIS	-	expression tag	UNP A6YEI0
A	-109	HIS	-	expression tag	UNP A6YEI0
A	-108	HIS	-	expression tag	UNP A6YEI0
A	-107	HIS	-	expression tag	UNP A6YEI0
A	-106	SER	-	expression tag	UNP A6YEI0
A	-105	SER	-	expression tag	UNP A6YEI0
A	-104	GLY	-	expression tag	UNP A6YEI0
A	-103	LEU	-	expression tag	UNP A6YEI0
A	-102	VAL	-	expression tag	UNP A6YEI0
A	-101	PRO	-	expression tag	UNP A6YEI0
A	-100	ARG	-	expression tag	UNP A6YEI0
A	-99	GLY	-	expression tag	UNP A6YEI0
A	-98	SER	-	expression tag	UNP A6YEI0
A	-97	HIS	-	expression tag	UNP A6YEI0
B	-116	MET	-	initiating methionine	UNP A6YEI0
B	-115	GLY	-	expression tag	UNP A6YEI0
B	-114	SER	-	expression tag	UNP A6YEI0
B	-113	SER	-	expression tag	UNP A6YEI0
B	-112	HIS	-	expression tag	UNP A6YEI0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-111	HIS	-	expression tag	UNP A6YEI0
B	-110	HIS	-	expression tag	UNP A6YEI0
B	-109	HIS	-	expression tag	UNP A6YEI0
B	-108	HIS	-	expression tag	UNP A6YEI0
B	-107	HIS	-	expression tag	UNP A6YEI0
B	-106	SER	-	expression tag	UNP A6YEI0
B	-105	SER	-	expression tag	UNP A6YEI0
B	-104	GLY	-	expression tag	UNP A6YEI0
B	-103	LEU	-	expression tag	UNP A6YEI0
B	-102	VAL	-	expression tag	UNP A6YEI0
B	-101	PRO	-	expression tag	UNP A6YEI0
B	-100	ARG	-	expression tag	UNP A6YEI0
B	-99	GLY	-	expression tag	UNP A6YEI0
B	-98	SER	-	expression tag	UNP A6YEI0
B	-97	HIS	-	expression tag	UNP A6YEI0

- Molecule 2 is 3,6,9,12,15-PENTAOXAHEPTADECAN-1-OL (CCD ID: AE4) (formula: $C_{12}H_{26}O_6$) (labeled as "Ligand of Interest" by depositor).



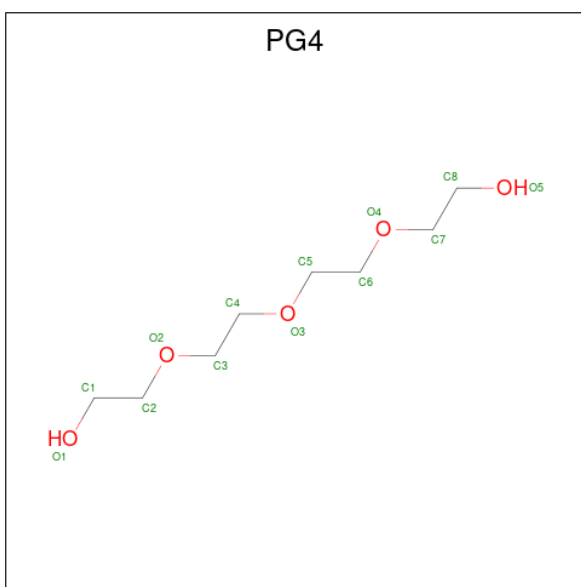
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	12	6		
2	B	1	Total	C	O	0	0
			18	12	6		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



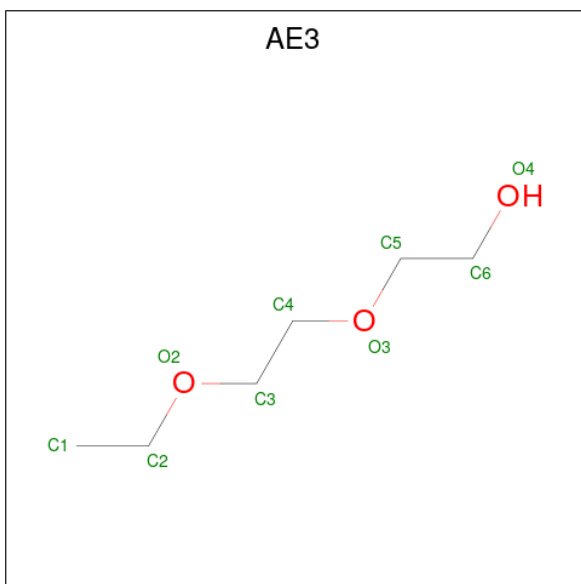
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	8	5		

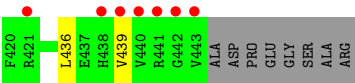
- Molecule 5 is 2-(2-ETHOXYETHOXY)ETHANOL (CCD ID: AE3) (formula: $C_6H_{14}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	75	Total 75	O 75	0	0
6	B	55	Total 55	O 55	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.89Å 129.52Å 61.31Å 90.00° 95.15° 90.00°	Depositor
Resolution (Å)	27.65 – 2.17 27.65 – 2.17	Depositor EDS
% Data completeness (in resolution range)	94.4 (27.65-2.17) 94.4 (27.65-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.215 , 0.246 0.221 , 0.252	Depositor DCC
R_{free} test set	3301 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6862	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AE4, AE3, PG4, PEG

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	0.52	0/3442	1.00	5/4709 (0.1%)
1	B	0.52	0/3355	1.02	6/4591 (0.1%)
All	All	0.52	0/6797	1.01	11/9300 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	GLU	N-CA-CB	-6.41	102.03	110.88
1	A	283	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	238	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	235	GLU	CB-CA-C	5.51	118.63	109.38
1	B	416	ARG	CB-CA-C	-5.45	103.82	110.08
1	B	257	THR	CA-CB-OG1	-5.25	101.72	109.60
1	B	169	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	239	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	335	LEU	N-CA-CB	-5.19	102.49	110.12
1	A	34	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	416	ARG	CB-CA-C	-5.13	104.18	110.08

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	277	ARG	Sidechain
1	A	393	ARG	Sidechain
1	B	277	ARG	Sidechain

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	3362	0	3355	26	0
1	B	3277	0	3266	37	0
2	A	18	0	26	6	0
2	B	18	0	26	5	0
3	A	21	0	30	3	0
3	B	14	0	20	0	0
4	B	13	0	18	5	0
5	B	9	0	14	0	0
6	A	75	0	0	2	0
6	B	55	0	0	1	0
All	All	6862	0	6755	63	0

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

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:GLN:HE22	4:B:603:PG4:H21	1.49	0.76
1:A:291:ALA:H	2:A:601:AE4:C9	2.05	0.68
1:B:214:ARG:HD2	1:B:334:GLU:HG2	1.79	0.65
1:B:50:GLY:O	1:B:142:ARG:HA	1.97	0.63
1:B:187:VAL:HG22	1:B:191[A]:ASP:OD2	1.98	0.63
1:B:266:PHE:CZ	1:B:439:VAL:HG12	2.35	0.62
1:A:291:ALA:H	2:A:601:AE4:H9C1	1.64	0.61
1:A:277:ARG:HD2	3:A:602:PEG:H22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:PRO:HG3	1:A:83:VAL:HG13	1.85	0.58
1:B:386:GLN:NE2	4:B:603:PG4:H52	2.18	0.58
1:A:353:ARG:HH12	1:A:361:LEU:H	1.51	0.57
1:A:336:VAL:HG22	2:A:601:AE4:H5C2	1.87	0.56
1:B:386:GLN:HE21	4:B:603:PG4:H52	1.71	0.56
1:B:161:ASP:HA	1:B:371:PHE:CZ	2.42	0.55
1:B:20:PRO:HG3	1:B:83:VAL:HG13	1.88	0.55
1:A:161:ASP:HA	1:A:371:PHE:CZ	2.42	0.55
1:A:291:ALA:H	2:A:601:AE4:H9C2	1.71	0.55
1:A:434:VAL:HG12	3:A:602:PEG:H32	1.89	0.55
1:A:115[B]:ARG:NH1	6:A:701:HOH:O	2.09	0.54
1:A:335:LEU:C	1:A:335:LEU:HD23	2.34	0.52
1:B:214:ARG:CD	1:B:334:GLU:HG2	2.40	0.52
1:B:386:GLN:NE2	4:B:603:PG4:H32	2.26	0.51
1:B:262:THR:HG22	1:B:265:THR:OG1	2.11	0.51
1:B:290:VAL:HA	2:B:601:AE4:H9C2	1.93	0.50
1:A:184:PRO:HG2	1:B:186:ALA:HB1	1.93	0.50
1:B:326:GLU:HB2	1:B:329:ARG:NH2	2.26	0.50
1:A:415:TYR:CG	1:A:425:VAL:HG21	2.47	0.49
1:B:386:GLN:HE21	4:B:603:PG4:H32	1.77	0.49
1:A:54:PRO:HB3	1:A:97:VAL:HG11	1.93	0.49
1:B:259:PHE:CZ	1:B:322:ARG:CD	2.96	0.49
1:A:291:ALA:HB2	2:A:601:AE4:H111	1.95	0.49
1:B:364:VAL:HG22	1:B:399:LEU:HB2	1.94	0.48
1:A:264:LEU:HA	1:A:368:VAL:HG21	1.96	0.48
1:A:290:VAL:HA	2:A:601:AE4:H9C1	1.96	0.48
1:A:364:VAL:HA	1:A:399:LEU:O	2.13	0.47
1:A:228:PRO:HA	1:A:418:SER:O	2.15	0.47
1:B:187:VAL:HG22	1:B:191[A]:ASP:CG	2.40	0.47
1:A:69:GLU:HB2	1:A:87:VAL:HG11	1.98	0.46
1:B:315:LEU:HD23	1:B:324:LEU:HD21	1.98	0.46
1:B:245:PRO:O	1:B:248:LEU:N	2.49	0.45
1:A:237:GLY:HA3	1:A:393:ARG:O	2.16	0.45
1:B:108:ARG:HD2	1:B:139:LEU:O	2.16	0.45
1:B:143:ARG:HH21	1:B:143:ARG:HG3	1.81	0.45
1:B:336:VAL:HG22	2:B:601:AE4:H3C2	1.99	0.44
1:B:259:PHE:CZ	1:B:322:ARG:HD3	2.53	0.44
1:A:105:ALA:HB3	1:A:106:PRO:HD3	2.00	0.44
1:B:409:LEU:HD21	1:B:436:LEU:HD21	2.01	0.43
1:A:396:LYS:HE2	3:A:604:PEG:H12	2.01	0.42
1:B:368:VAL:O	1:B:403:VAL:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LEU:HD11	1:A:163:LEU:HD21	2.01	0.42
2:B:601:AE4:H172	6:B:736:HOH:O	2.18	0.42
1:B:290:VAL:HA	2:B:601:AE4:C9	2.50	0.42
1:B:291:ALA:H	2:B:601:AE4:H8C1	1.84	0.42
1:A:407:ASP:N	6:A:704:HOH:O	2.53	0.42
1:B:71:LEU:HD11	1:B:163:LEU:HD21	2.00	0.42
1:B:372:ASP:OD2	1:B:410:ARG:NH1	2.53	0.41
1:B:332:VAL:O	1:B:336:VAL:HG23	2.20	0.41
1:B:43:THR:HA	1:B:148:LEU:O	2.21	0.41
1:B:364:VAL:HA	1:B:399:LEU:O	2.20	0.41
1:A:43:THR:HA	1:A:148:LEU:O	2.21	0.41
1:B:244:ALA:HB3	1:B:409:LEU:HB3	2.03	0.41
1:B:161:ASP:OD1	1:B:371:PHE:CE1	2.74	0.40
1:B:259:PHE:HZ	1:B:322:ARG:HD3	1.87	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	429/568 (76%)	421 (98%)	8 (2%)	0	100	100
1	B	416/568 (73%)	402 (97%)	14 (3%)	0	100	100
All	All	845/1136 (74%)	823 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/449 (78%)	342 (98%)	8 (2%)	44	56
1	B	343/449 (76%)	334 (97%)	9 (3%)	40	51
All	All	693/898 (77%)	676 (98%)	17 (2%)	42	53

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLU
1	A	118	LEU
1	A	230	ASP
1	A	335	LEU
1	A	353	ARG
1	A	358	ARG
1	A	393	ARG
1	A	443	VAL
1	B	29	LEU
1	B	118	LEU
1	B	202	SER
1	B	252	VAL
1	B	262	THR
1	B	335	LEU
1	B	359	VAL
1	B	368	VAL
1	B	369	GLN

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

Mol	Chain	Res	Type
1	A	152	HIS
1	A	339	GLN
1	B	152	HIS
1	B	339	GLN
1	B	386	GLN
1	B	438	HIS

5.3.3 RNA ⓘ

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](#)

9 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	PEG	A	602	-	6,6,6	0.21	0	5,5,5	0.21	0
3	PEG	B	602	-	6,6,6	0.21	0	5,5,5	0.06	0
3	PEG	B	604	-	6,6,6	0.33	0	5,5,5	0.16	0
4	PG4	B	603	-	12,12,12	0.29	0	11,11,11	0.22	0
2	AE4	A	601	-	17,17,17	0.21	0	16,16,16	0.18	0
3	PEG	A	604	-	6,6,6	0.19	0	5,5,5	0.16	0
3	PEG	A	605	-	6,6,6	0.18	0	5,5,5	0.13	0
5	AE3	B	605	-	8,8,8	1.66	2 (25%)	7,7,7	0.92	0
2	AE4	B	601	-	17,17,17	0.16	0	16,16,16	0.26	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	PEG	A	602	-	-	3/4/4/4	-
3	PEG	B	602	-	-	1/4/4/4	-
3	PEG	B	604	-	-	2/4/4/4	-
4	PG4	B	603	-	-	6/10/10/10	-
2	AE4	A	601	-	-	7/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	604	-	-	2/4/4/4	-
3	PEG	A	605	-	-	2/4/4/4	-
5	AE3	B	605	-	-	2/6/6/6	-
2	AE4	B	601	-	-	7/15/15/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	605	AE3	C4-C3	2.78	1.63	1.49
5	B	605	AE3	C1-C2	2.39	1.64	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	AE4	O4-C5-C6-O7
2	B	601	AE4	O13-C14-C15-O16
3	A	605	PEG	O2-C3-C4-O4
2	B	601	AE4	O10-C11-C12-O13
2	B	601	AE4	O16-C17-C18-O19
2	A	601	AE4	O13-C14-C15-O16
3	B	604	PEG	O1-C1-C2-O2
2	B	601	AE4	O7-C8-C9-O10
3	A	602	PEG	O1-C1-C2-O2
3	A	604	PEG	O2-C3-C4-O4
3	A	605	PEG	O1-C1-C2-O2
3	B	602	PEG	O2-C3-C4-O4
2	B	601	AE4	O4-C5-C6-O7
2	A	601	AE4	O10-C11-C12-O13
5	B	605	AE3	O2-C3-C4-O3
2	B	601	AE4	C15-C14-O13-C12
4	B	603	PG4	C1-C2-O2-C3
2	A	601	AE4	C9-C8-O7-C6
2	A	601	AE4	C14-C15-O16-C17
3	A	602	PEG	C1-C2-O2-C3
3	A	602	PEG	O2-C3-C4-O4
5	B	605	AE3	C4-C3-O2-C2
2	B	601	AE4	C2-C3-O4-C5
3	B	604	PEG	C1-C2-O2-C3

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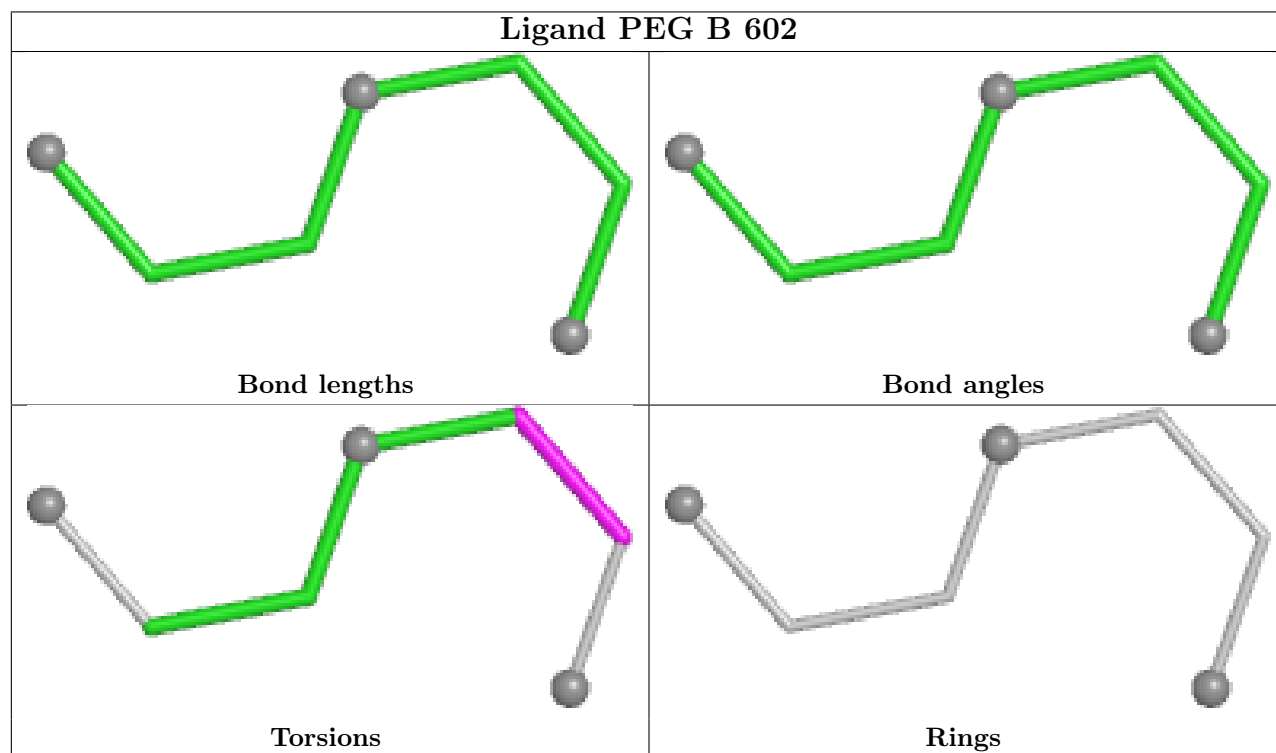
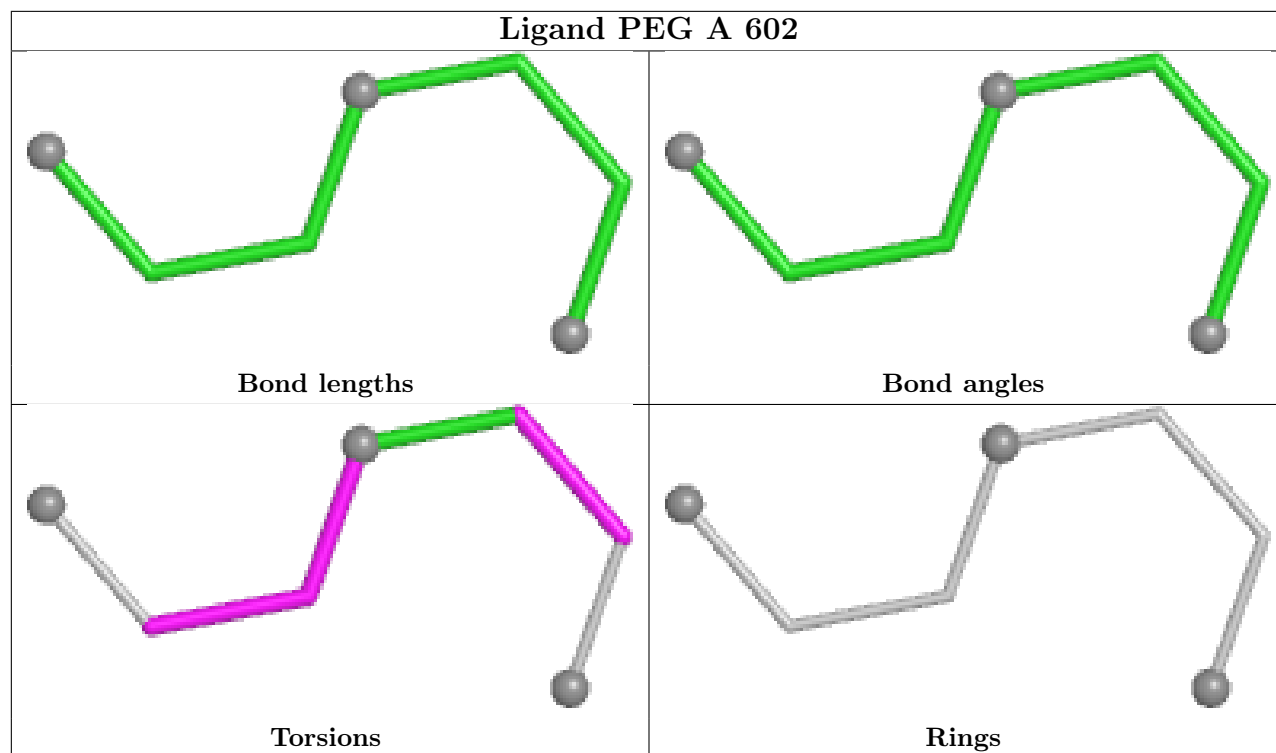
Mol	Chain	Res	Type	Atoms
4	B	603	PG4	O4-C7-C8-O5
4	B	603	PG4	C4-C3-O2-C2
2	A	601	AE4	C2-C3-O4-C5
4	B	603	PG4	O2-C3-C4-O3
4	B	603	PG4	C3-C4-O3-C5
2	A	601	AE4	C6-C5-O4-C3
3	A	604	PEG	C1-C2-O2-C3
4	B	603	PG4	O3-C5-C6-O4

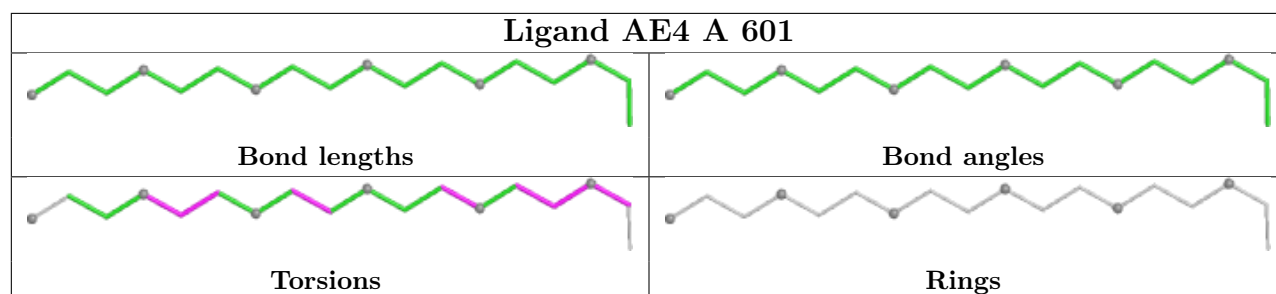
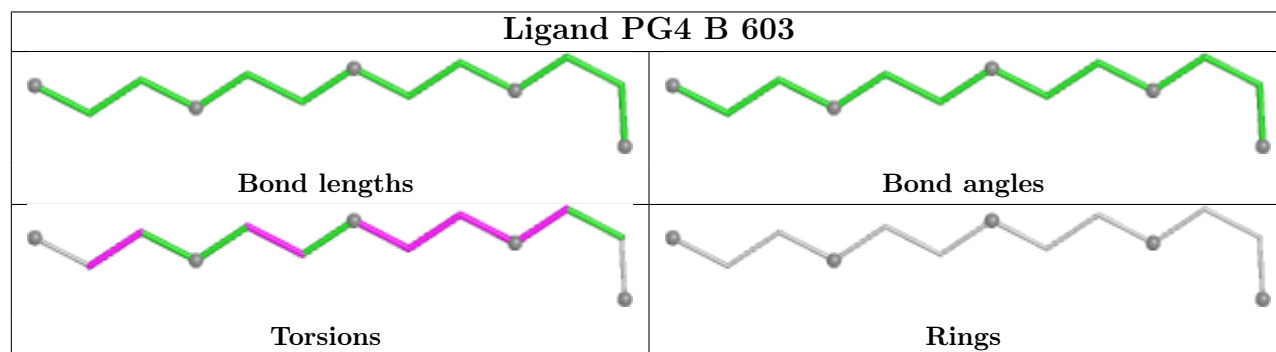
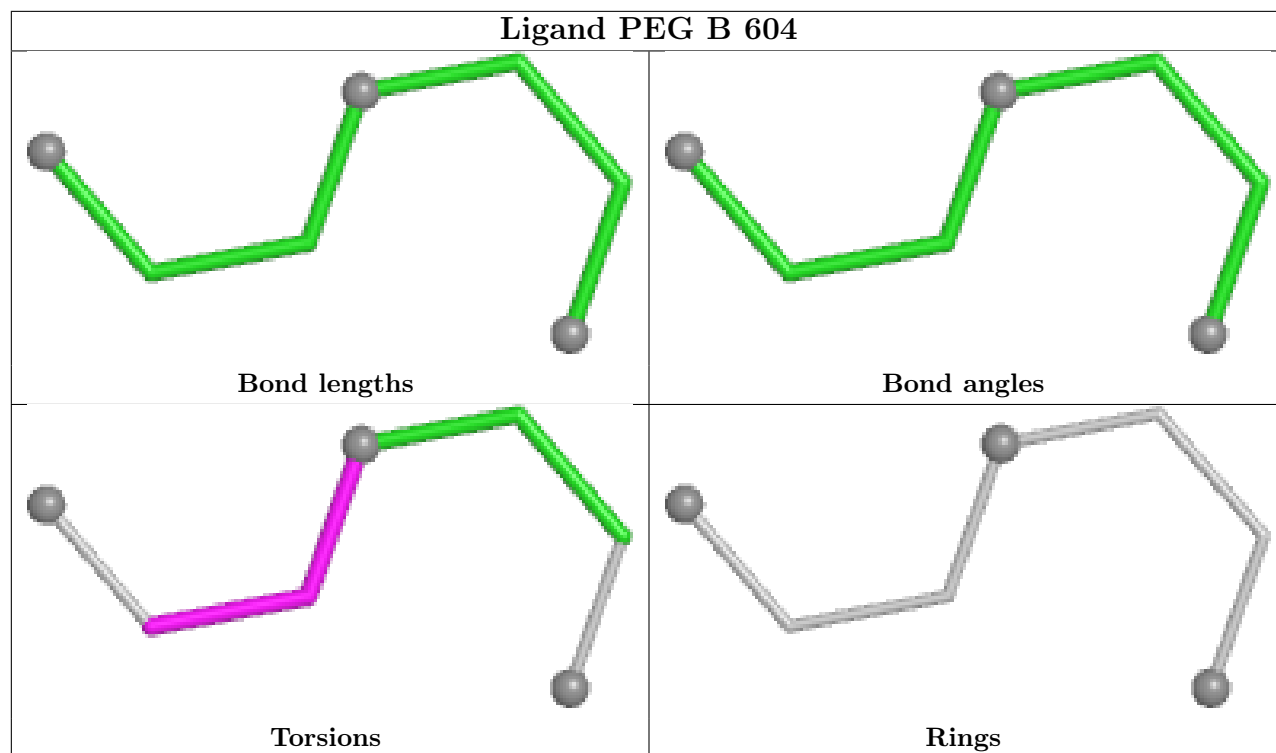
There are no ring outliers.

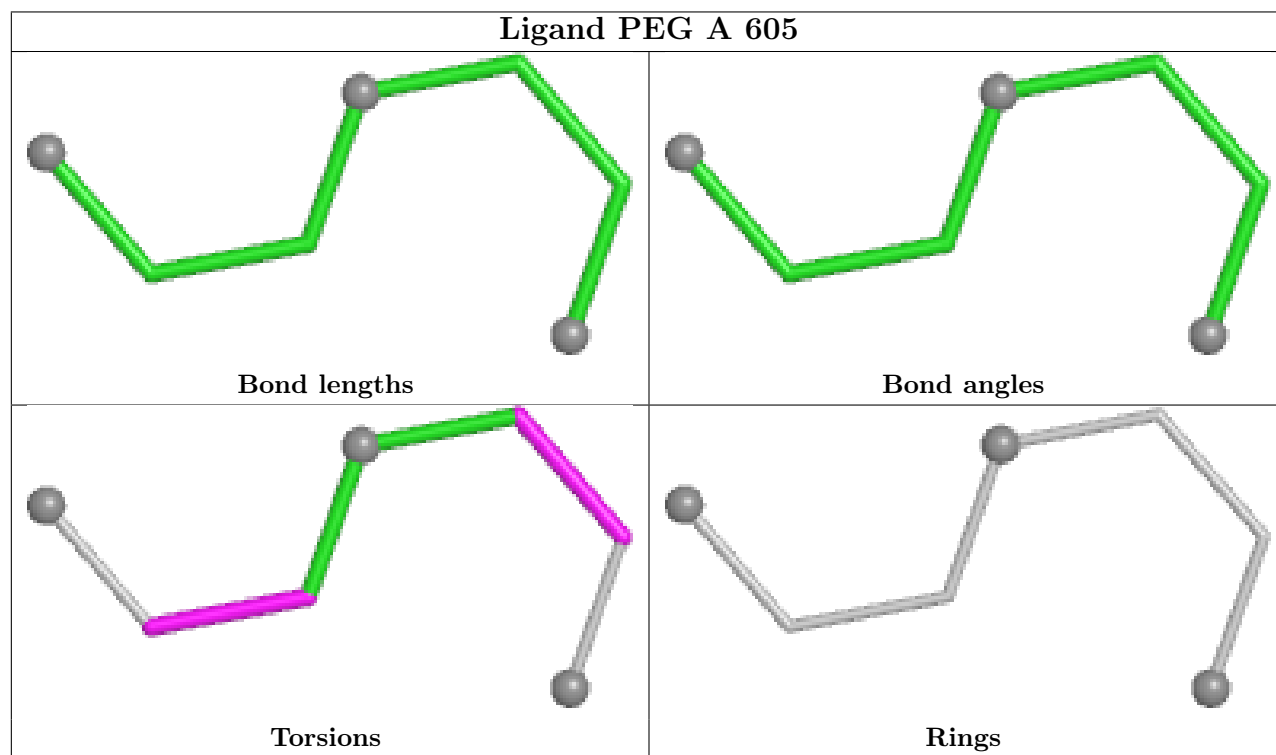
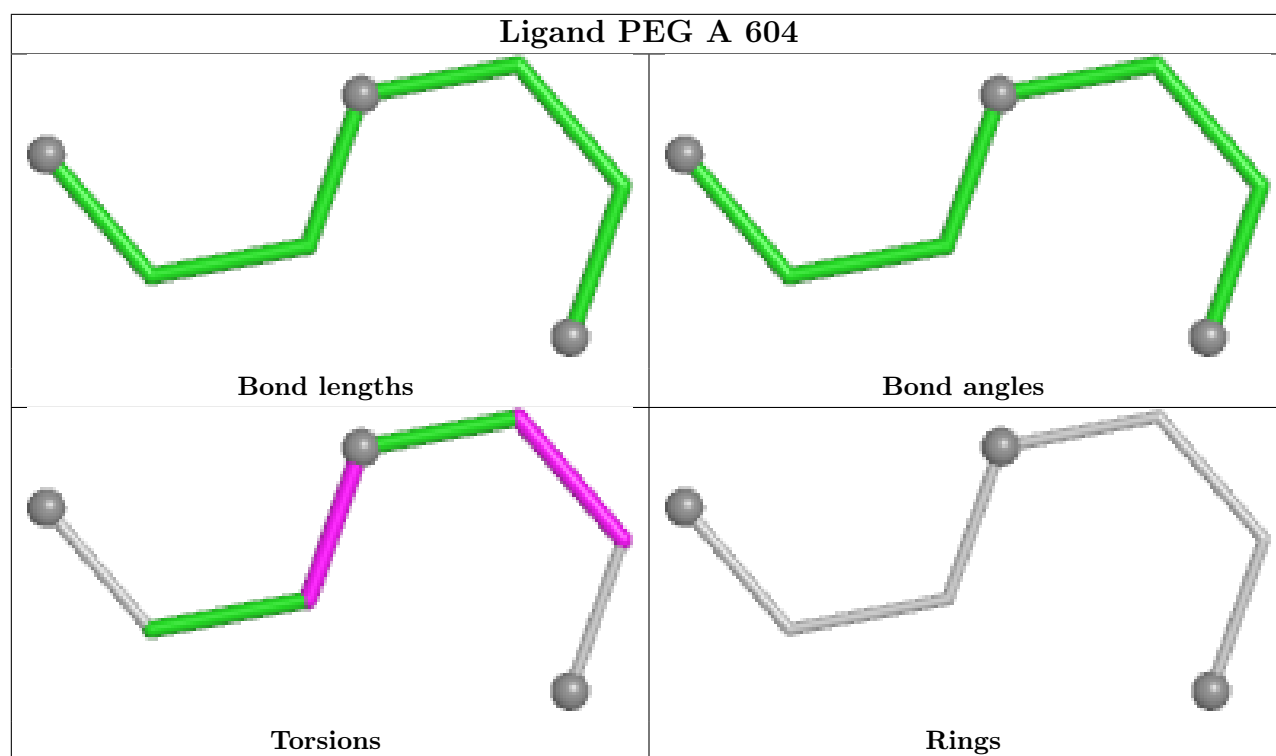
5 monomers are involved in 19 short contacts:

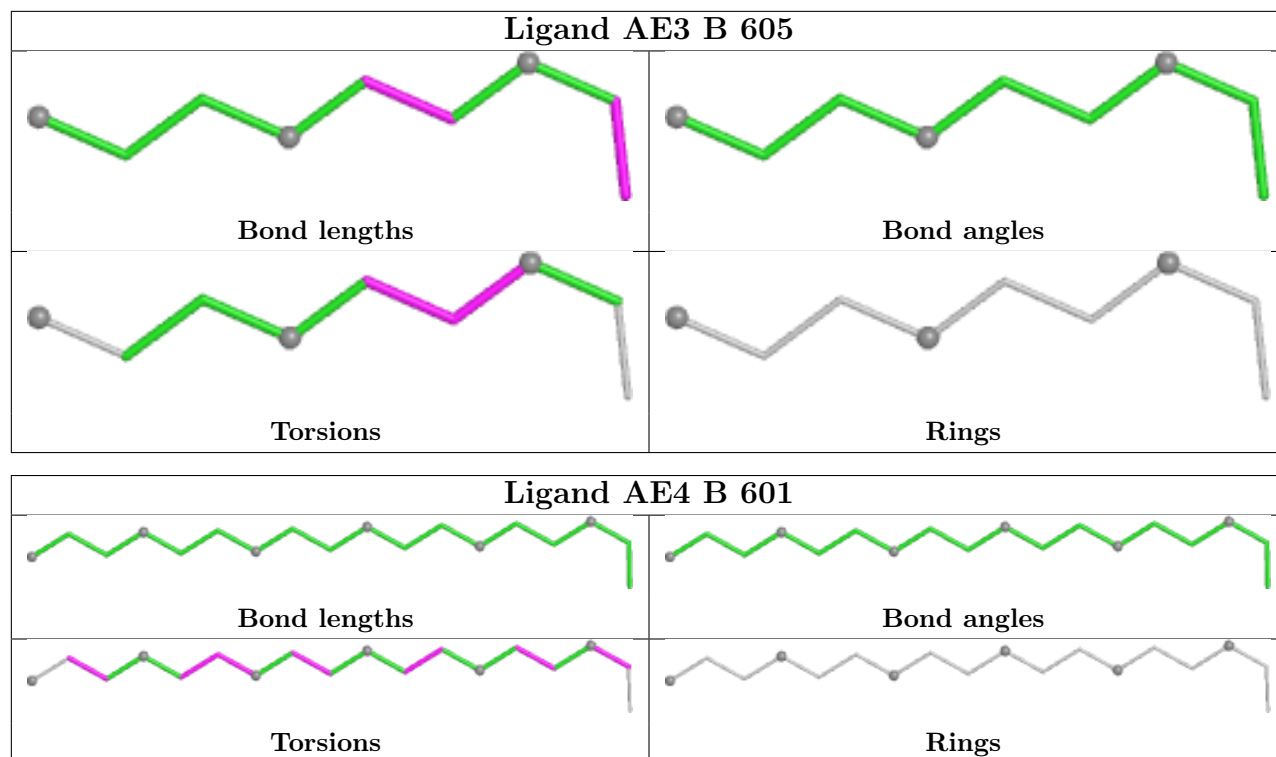
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	PEG	2	0
4	B	603	PG4	5	0
2	A	601	AE4	6	0
3	A	604	PEG	1	0
2	B	601	AE4	5	0

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	430/568 (75%)	0.30	28 (6%) 25 24	16, 31, 57, 119	1 (0%)
1	B	419/568 (73%)	0.87	79 (18%) 3 3	20, 37, 75, 99	1 (0%)
All	All	849/1136 (74%)	0.58	107 (12%) 8 7	16, 34, 70, 119	2 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	ALA	8.8
1	A	357	THR	7.1
1	B	255	ALA	6.9
1	B	442	GLY	6.2
1	B	443	VAL	6.1
1	A	358	ARG	6.0
1	A	17	ASP	6.0
1	B	408	GLY	5.9
1	B	440	VAL	5.8
1	B	359	VAL	5.3
1	B	184	PRO	5.2
1	A	352	ALA	5.2
1	A	356	GLY	4.8
1	B	250	ALA	4.8
1	B	252	VAL	4.7
1	B	233	ALA	4.7
1	A	91	ALA	4.7
1	B	110	ARG	4.7
1	A	446	PRO	4.6
1	B	259	PHE	4.5
1	B	247	GLY	4.5
1	B	249	ALA	4.4
1	B	234	HIS	4.4
1	A	354	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	186	ALA	4.3
1	B	260	GLY	4.3
1	A	406	THR	4.3
1	B	246	PRO	4.2
1	B	406	THR	4.1
1	B	371	PHE	4.1
1	B	439	VAL	4.1
1	B	321	VAL	3.9
1	B	368	VAL	3.9
1	B	390	PRO	3.9
1	B	370	ASN	3.8
1	B	229	VAL	3.7
1	A	353	ARG	3.7
1	B	404	SER	3.6
1	B	254	ARG	3.6
1	B	393	ARG	3.6
1	B	441	ARG	3.6
1	B	396	LYS	3.5
1	B	251	ALA	3.5
1	B	256	ARG	3.5
1	A	370	ASN	3.5
1	B	257	THR	3.5
1	B	318	THR	3.5
1	B	392	GLU	3.4
1	B	407	ASP	3.4
1	B	226	VAL	3.3
1	B	317	GLY	3.3
1	B	438	HIS	3.3
1	B	248	LEU	3.2
1	A	184	PRO	3.2
1	B	231	VAL	3.1
1	B	105	ALA	3.1
1	B	323	VAL	3.1
1	B	405	ASP	3.0
1	B	421	ARG	3.0
1	B	261	HIS	3.0
1	A	186	ALA	2.9
1	B	324	LEU	2.9
1	B	228	PRO	2.9
1	B	329	ARG	2.8
1	B	315	LEU	2.8
1	B	232	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	326	GLU	2.8
1	A	393	ARG	2.7
1	B	266	PHE	2.7
1	A	176	ALA	2.7
1	B	320	ASP	2.7
1	A	407	ASP	2.7
1	B	101	ALA	2.7
1	B	391	PRO	2.6
1	B	409	LEU	2.6
1	B	322	ARG	2.6
1	B	369	GLN	2.6
1	B	220	ALA	2.6
1	B	103	PHE	2.6
1	A	445	ASP	2.5
1	B	351	GLY	2.5
1	A	391	PRO	2.5
1	B	183	PRO	2.5
1	B	213	ARG	2.4
1	B	107	VAL	2.4
1	A	79	ASP	2.4
1	B	262	THR	2.4
1	B	419	LEU	2.3
1	A	258	SER	2.3
1	B	91	ALA	2.3
1	A	392	GLU	2.3
1	B	187	VAL	2.3
1	A	92	ALA	2.3
1	A	351	GLY	2.3
1	B	253	GLU	2.3
1	B	143	ARG	2.3
1	B	294	ALA	2.2
1	B	235	GLU	2.2
1	B	395	SER	2.2
1	A	177	GLY	2.2
1	B	140	ALA	2.2
1	B	185	PRO	2.1
1	A	369	GLN	2.1
1	B	319	SER	2.1
1	A	175	LEU	2.0
1	B	216	ALA	2.0
1	A	408	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

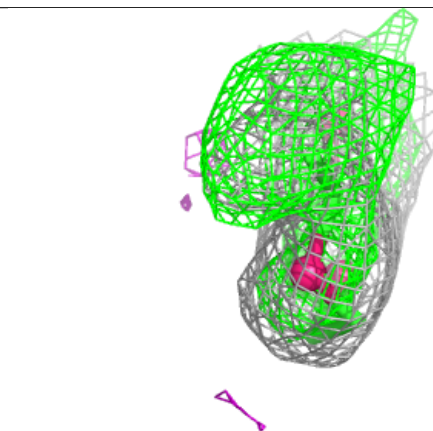
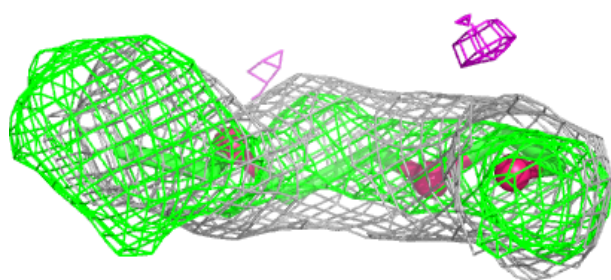
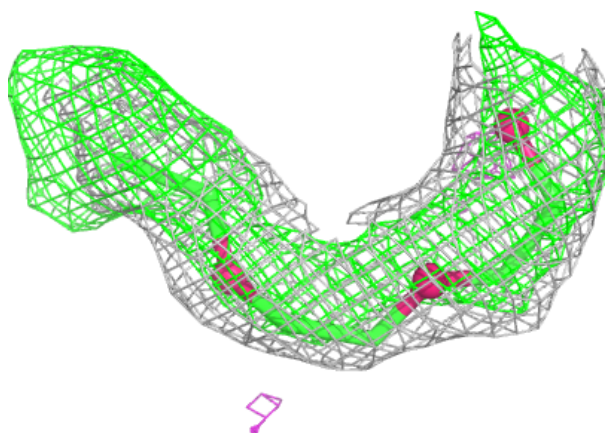
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	AE3	B	605	9/9	0.73	0.57	106,116,130,134	0
2	AE4	B	601	18/18	0.78	0.16	46,52,58,58	0
3	PEG	B	604	7/7	0.79	0.19	48,48,50,51	0
2	AE4	A	601	18/18	0.82	0.17	37,48,54,55	0
4	PG4	B	603	13/13	0.83	0.14	48,52,55,56	0
3	PEG	A	604	7/7	0.85	0.13	48,50,54,55	0
3	PEG	B	602	7/7	0.87	0.13	37,39,51,53	0
3	PEG	A	602	7/7	0.90	0.12	33,35,38,41	0
3	PEG	A	605	7/7	0.91	0.12	41,43,51,52	0

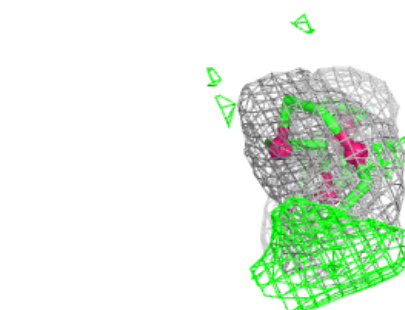
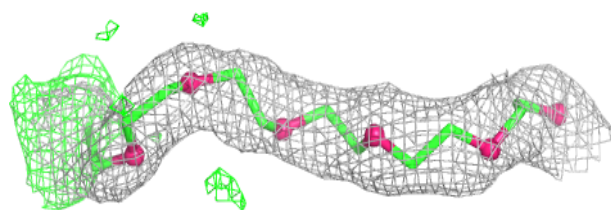
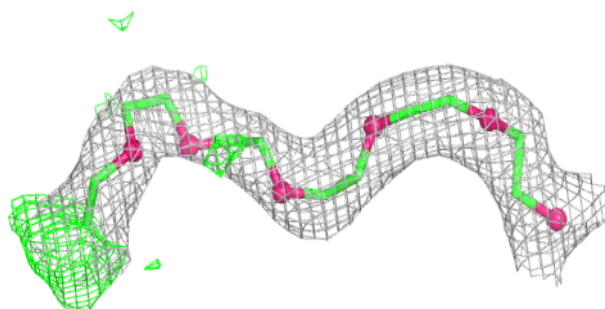
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AE3 B 605:

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

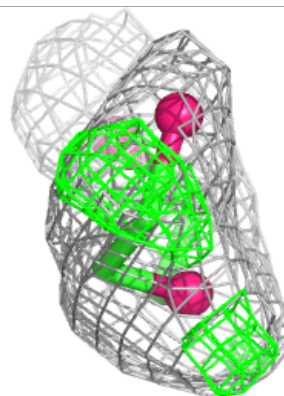
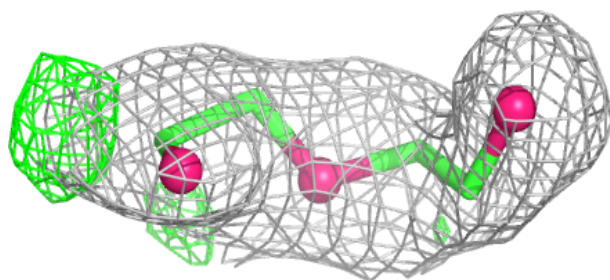
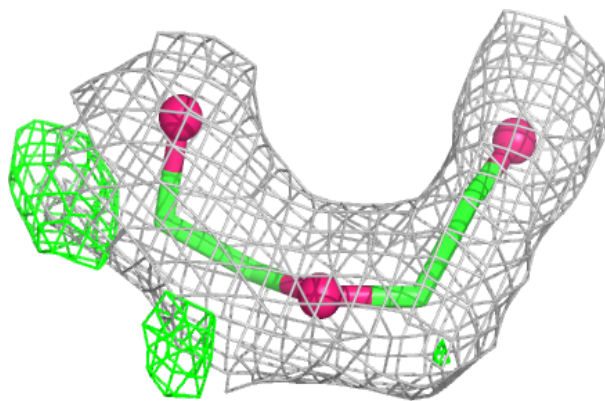
**Electron density around AE4 B 601:**

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

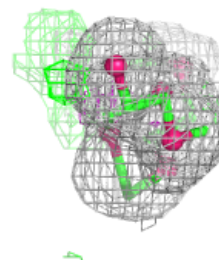
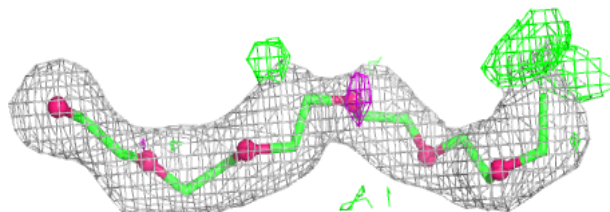
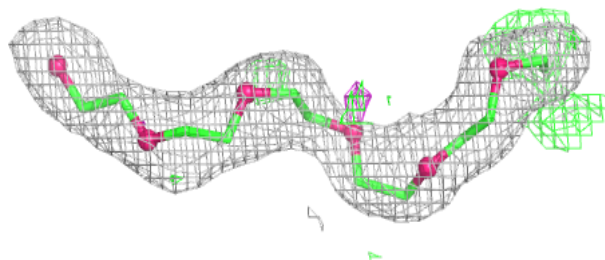


Electron density around PEG B 604:

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

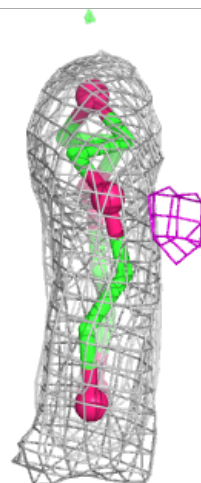
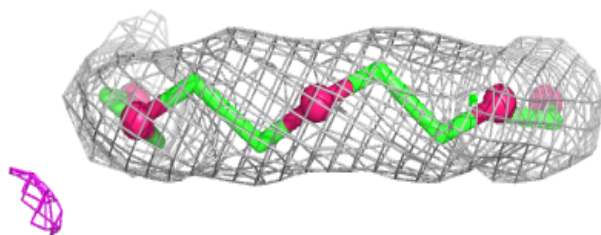
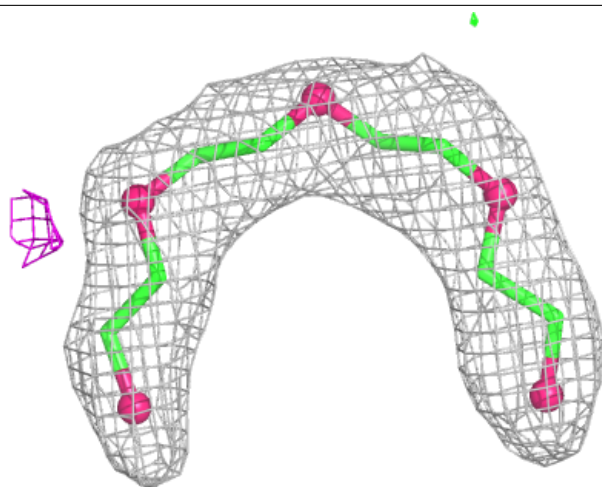
**Electron density around AE4 A 601:**

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



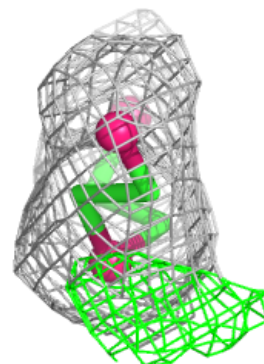
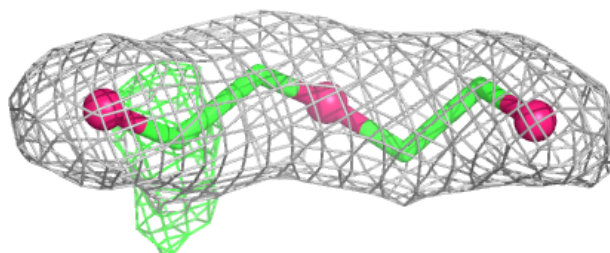
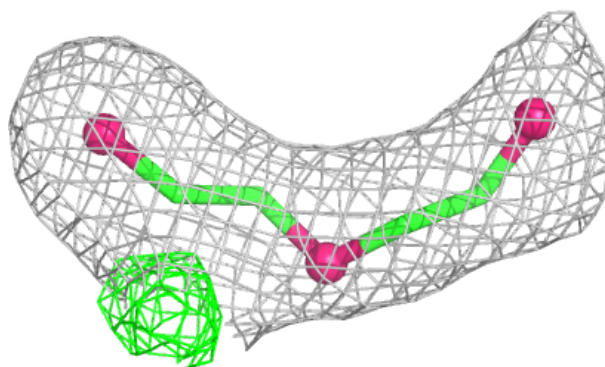
Electron density around PG4 B 603:

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and green (positive)

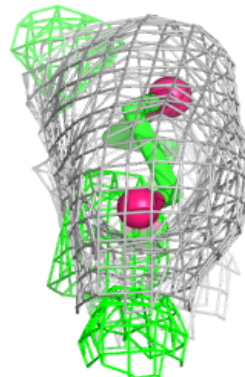
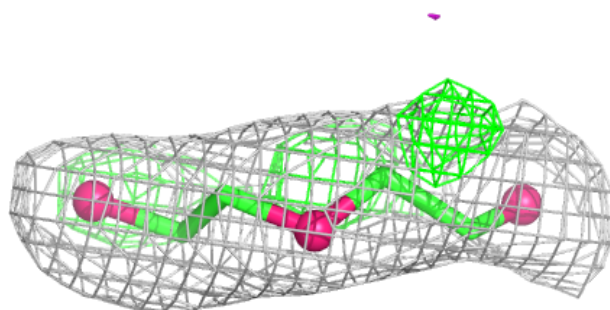
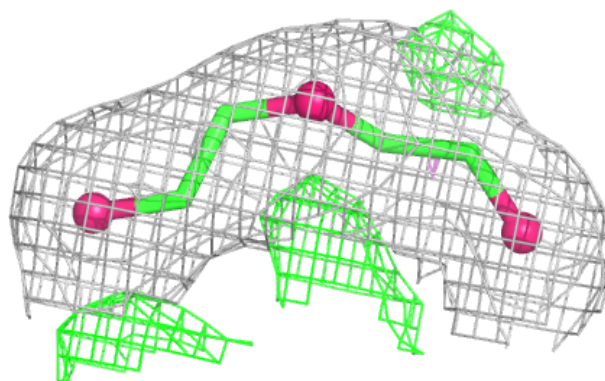


Electron density around PEG A 604:

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

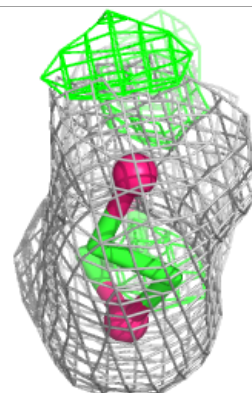
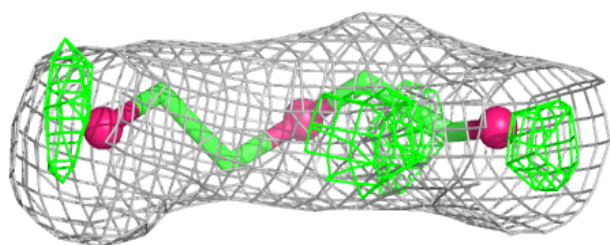
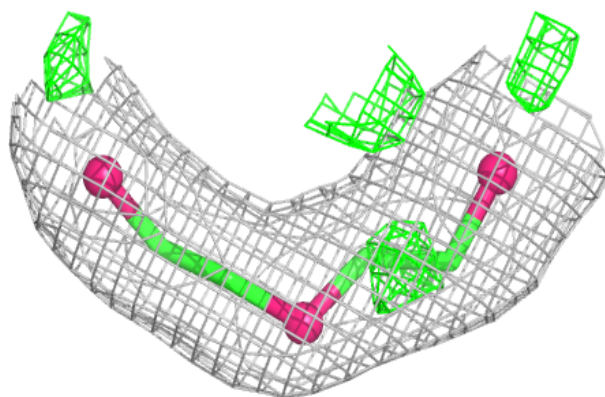
**Electron density around PEG B 602:**

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

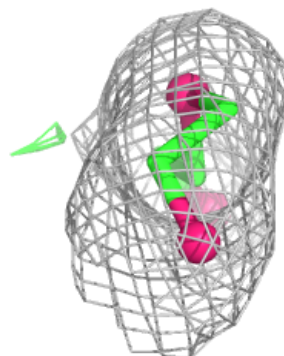
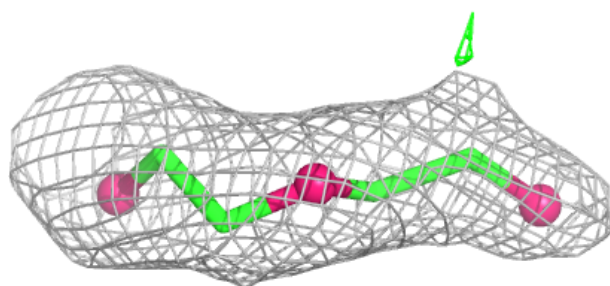
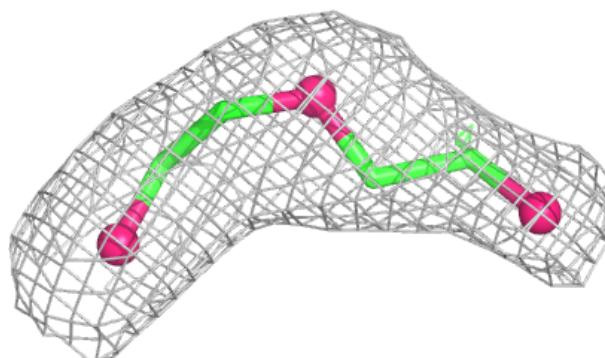


Electron density around PEG A 602:

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

**Electron density around PEG A 605:**

$2mF_o-DF_c$ (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.