



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:29 PM UTC

PDB ID : 8RM3 / pdb_00008rm3
Title : Crystal structure of ferrioxamine transporter FoxA
Authors : Josts, I.; Tidow, H.; Mislin, G.
Deposited on : 2024-01-04
Resolution : 2.22 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

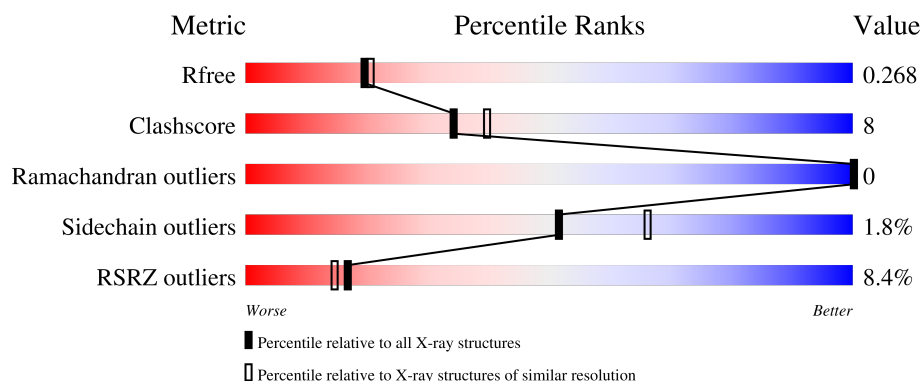
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	820	

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	DMS	A	909	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5668 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 Ferrioxamine receptor FoxA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	677	5325	3345	910	1059	11	0	0	0

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



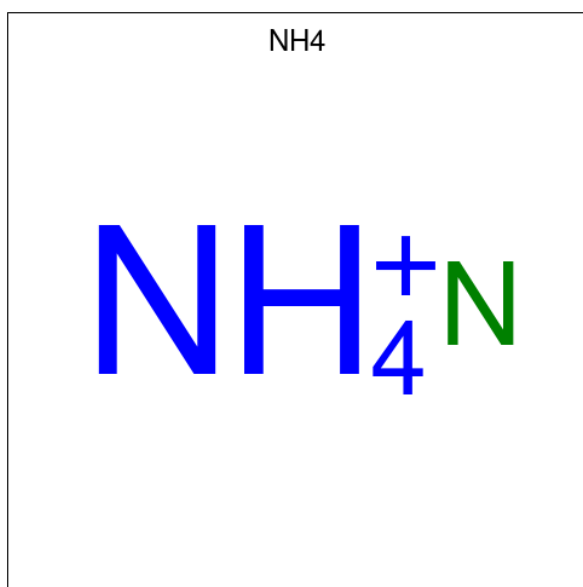
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			9	8	1		
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is AMMONIUM ION (CCD ID: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	N	0	0
			1	1		

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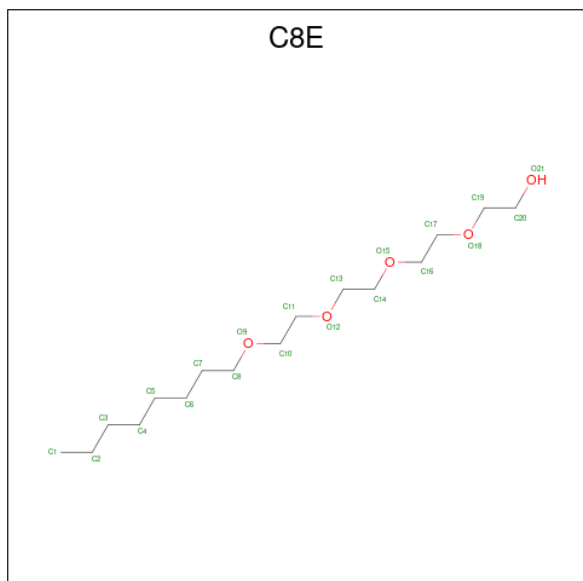
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N		0	0
			1	1			

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	9	1		
6	A	1	Total	C	O	0	0
			10	9	1		
6	A	1	Total	C	O	0	0
			21	16	5		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

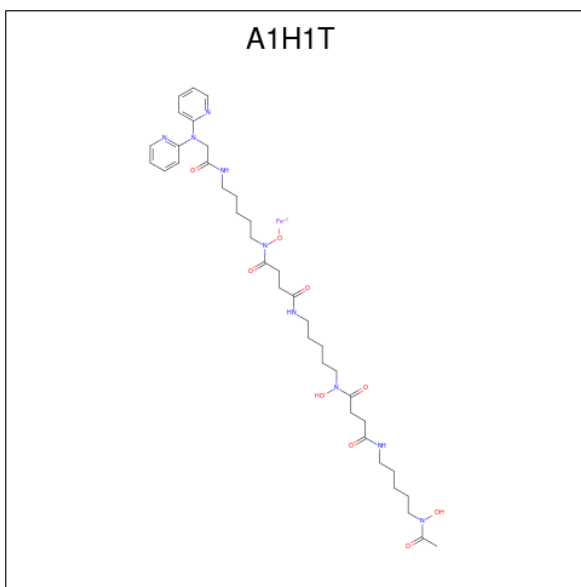


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Na	0	0
			1	1		

- Molecule 9 is [5-[2-(dipyridin-2-ylamino)ethanoylamino]pentyl-[4-[5-[[4-[5-[ethanoyl(oxidanyl)amino]pentylamino]-4-oxidanylidene-butanoyl]-oxidanyl-amino]pentylamino]-4-oxidanylidene-butanoyl]amino]oxyiron (CCD ID: A1H1T) (formula: C₃₇H₅₆FeN₉O₉) (labeled as "Ligand of Interest" by depositor).

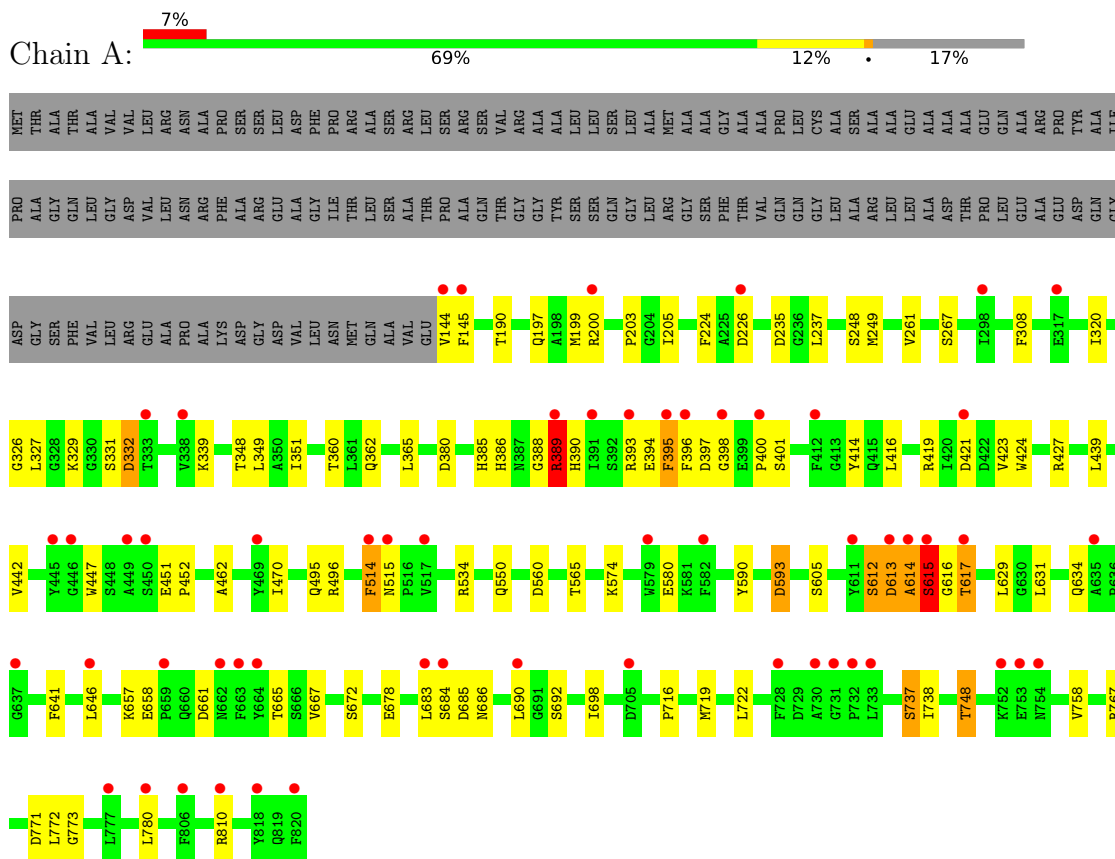


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
9	A	1	56	37	1	9	9	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	137	Total	O	0	0
			137	137		

- Molecule 1: Ferrioxamine receptor FoxA



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.03Å 94.03Å 178.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	81.43 – 2.22 81.43 – 2.22	Depositor EDS
% Data completeness (in resolution range)	83.0 (81.43-2.22) 83.0 (81.43-2.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.222 , 0.258 0.226 , 0.268	Depositor DCC
R_{free} test set	1820 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5668	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: BOG, A1H1T, GOL, SO4, C8E, DMS, NH4, NA

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	0.61	2/5451 (0.0%)	0.92	9/7397 (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	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	614	ALA	N-CA	-6.34	1.38	1.46
1	A	613	ASP	CA-C	-6.08	1.44	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	613	ASP	CA-C-N	-12.89	103.64	126.45
1	A	613	ASP	C-N-CA	-12.89	103.64	126.45
1	A	615	SER	N-CA-C	-12.13	98.76	113.19
1	A	613	ASP	O-C-N	9.17	134.63	122.43
1	A	389	ARG	N-CA-C	-7.64	104.10	113.19
1	A	395	PHE	CA-CB-CG	7.40	121.20	113.80
1	A	332	ASP	N-CA-C	-6.16	102.59	110.53
1	A	614	ALA	N-CA-C	-6.12	103.67	113.28
1	A	396	PHE	N-CA-CB	-5.35	102.71	110.36

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	389	ARG	Sidechain
1	A	393	ARG	Sidechain
1	A	419	ARG	Sidechain
1	A	496	ARG	Sidechain
1	A	534	ARG	Sidechain
1	A	810	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	5325	0	5038	81	0
2	A	69	0	101	1	0
3	A	18	0	24	1	0
4	A	2	0	0	0	0
5	A	4	0	6	4	0
6	A	41	0	68	2	0
7	A	15	0	0	0	0
8	A	1	0	0	0	0
9	A	56	0	0	0	0
10	A	137	0	0	1	0
All	All	5668	0	5237	82	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 8.

All (82) 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:613:ASP:O	1:A:614:ALA:HB3	1.70	0.90
1:A:197:GLN:O	1:A:200:ARG:NE	2.12	0.81
1:A:612:SER:C	1:A:614:ALA:H	1.92	0.76
1:A:612:SER:C	1:A:614:ALA:N	2.41	0.75
1:A:385:HIS:CE1	1:A:389:ARG:HG3	2.25	0.71
1:A:235:ASP:HA	3:A:914:GOL:H31	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:THR:HG21	1:A:574:LYS:HE3	1.74	0.70
1:A:331:SER:OG	1:A:332:ASP:O	2.09	0.69
1:A:613:ASP:O	1:A:614:ALA:CB	2.40	0.68
1:A:421:ASP:HB3	1:A:423:VAL:H	1.61	0.65
1:A:565:THR:CG2	1:A:574:LYS:HE3	2.28	0.64
1:A:631:LEU:HB2	6:A:913:C8E:H61	1.79	0.62
1:A:397:ASP:CG	1:A:398:GLY:H	2.10	0.60
1:A:190:THR:CB	1:A:200:ARG:HH22	2.15	0.59
1:A:205:ILE:HD11	1:A:261:VAL:HG11	1.85	0.58
1:A:614:ALA:C	1:A:616:GLY:N	2.61	0.58
1:A:199:MET:HE1	1:A:261:VAL:HG22	1.87	0.56
1:A:748:THR:HG22	1:A:758:VAL:HB	1.88	0.56
1:A:267:SER:HB2	1:A:605:SER:HA	1.87	0.56
1:A:613:ASP:OD2	1:A:617:THR:HG23	2.05	0.56
1:A:386:HIS:C	1:A:388:GLY:H	2.14	0.56
1:A:593:ASP:OD1	1:A:593:ASP:N	2.40	0.55
1:A:613:ASP:C	1:A:615:SER:H	2.15	0.55
1:A:629:LEU:HD12	6:A:913:C8E:H32	1.87	0.55
1:A:771:ASP:OD1	1:A:773:GLY:N	2.36	0.55
1:A:380:ASP:HB3	1:A:447:TRP:HE1	1.71	0.54
1:A:716:PRO:HG2	1:A:719:MET:HE2	1.90	0.53
1:A:226:ASP:H	5:A:909:DMS:H12	1.74	0.53
1:A:388:GLY:C	1:A:390:HIS:H	2.16	0.53
1:A:237:LEU:HD22	1:A:470:ILE:HG12	1.90	0.52
1:A:394:GLU:HG3	1:A:395:PHE:HD1	1.74	0.52
1:A:613:ASP:C	1:A:615:SER:N	2.66	0.52
1:A:614:ALA:C	1:A:616:GLY:H	2.15	0.52
1:A:190:THR:HB	1:A:200:ARG:HH22	1.75	0.52
1:A:388:GLY:C	1:A:390:HIS:N	2.68	0.52
1:A:737:SER:C	1:A:738:ILE:HD12	2.35	0.51
1:A:199:MET:HE3	1:A:205:ILE:HD13	1.93	0.51
1:A:550:GLN:HB2	1:A:590:TYR:CE1	2.46	0.50
1:A:672:SER:HB2	1:A:698:ILE:HD12	1.94	0.50
1:A:224:PHE:HD1	5:A:909:DMS:H13	1.79	0.48
1:A:737:SER:O	1:A:738:ILE:HD12	2.13	0.48
1:A:144:VAL:HG12	1:A:145:PHE:H	1.79	0.48
1:A:683:LEU:O	1:A:685:ASP:N	2.47	0.48
1:A:550:GLN:HB2	1:A:590:TYR:CZ	2.49	0.47
1:A:514:PHE:O	1:A:515:ASN:HB2	2.14	0.47
1:A:684:SER:C	1:A:686:ASN:H	2.22	0.47
1:A:646:LEU:HG	2:A:902:BOG:H8'1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:HIS:HB3	1:A:388:GLY:O	2.15	0.46
1:A:421:ASP:HB2	1:A:424:TRP:H	1.81	0.45
1:A:657:LYS:HE2	1:A:661:ASP:O	2.16	0.45
1:A:385:HIS:ND1	1:A:389:ARG:HA	2.31	0.45
1:A:397:ASP:CG	1:A:398:GLY:N	2.75	0.45
1:A:657:LYS:HG3	1:A:658:GLU:O	2.17	0.45
1:A:613:ASP:CG	1:A:617:THR:HG23	2.42	0.45
1:A:349:LEU:HD23	1:A:351:ILE:HD11	1.98	0.44
1:A:320:ILE:HG12	1:A:351:ILE:HG23	1.98	0.44
1:A:203:PRO:HG3	1:A:678:GLU:HB2	1.99	0.44
1:A:416:LEU:O	1:A:427:ARG:HA	2.18	0.44
1:A:327:LEU:HD21	1:A:329:LYS:HD3	1.98	0.44
1:A:439:LEU:HB3	1:A:462:ALA:HB3	1.99	0.44
1:A:560:ASP:O	1:A:580:GLU:HA	2.17	0.44
1:A:421:ASP:CB	1:A:424:TRP:H	2.31	0.43
1:A:665:THR:HG23	1:A:667:VAL:HG22	1.99	0.43
1:A:690:LEU:O	1:A:722:LEU:HA	2.18	0.43
1:A:565:THR:HG21	1:A:574:LYS:CE	2.47	0.42
1:A:224:PHE:CD1	5:A:909:DMS:H13	2.54	0.42
1:A:394:GLU:HG3	1:A:395:PHE:CD1	2.53	0.42
1:A:248:SER:C	1:A:249:MET:HE2	2.44	0.42
1:A:772:LEU:HB2	1:A:780:LEU:O	2.19	0.42
1:A:390:HIS:HB3	1:A:514:PHE:CE2	2.54	0.42
1:A:308:PHE:CE2	1:A:326:GLY:HA3	2.55	0.42
1:A:144:VAL:HG12	1:A:145:PHE:N	2.34	0.41
1:A:199:MET:HE1	1:A:261:VAL:CG2	2.51	0.41
1:A:360:THR:O	1:A:414:TYR:HA	2.21	0.41
1:A:451:GLU:HA	1:A:452:PRO:HD3	1.95	0.41
1:A:737:SER:HB2	1:A:767:ARG:HH12	1.85	0.41
1:A:400:PRO:O	1:A:401:SER:OG	2.32	0.41
1:A:470:ILE:HD12	1:A:495:GLN:HG2	2.02	0.41
1:A:634:GLN:HB2	1:A:641:PHE:HD1	1.85	0.41
1:A:339:LYS:HB2	1:A:339:LYS:HE2	1.77	0.41
1:A:348:THR:HG23	1:A:362:GLN:HG2	2.04	0.40
5:A:909:DMS:H11	10:A:1049:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	675/820 (82%)	649 (96%)	26 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	566/667 (85%)	556 (98%)	10 (2%)	51	66

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	LEU
1	A	442	VAL
1	A	514	PHE
1	A	593	ASP
1	A	612	SER
1	A	615	SER
1	A	617	THR
1	A	692	SER
1	A	737	SER
1	A	748	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	370	ASN
1	A	415	GLN
1	A	634	GLN
1	A	651	GLN
1	A	710	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 2 are modelled with single atom and 1 is monoatomic - leaving 15 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	$\# Z > 2$
6	C8E	A	913	-	20,20,20	0.39	0	19,19,19	0.35	0
2	BOG	A	903	-	8,8,20	0.27	0	7,7,25	0.31	0
6	C8E	A	911	-	9,9,20	0.39	0	8,8,19	0.25	0
3	GOL	A	914	-	5,5,5	0.51	0	5,5,5	0.75	0
7	SO4	A	918	-	4,4,4	0.79	0	6,6,6	0.22	0
2	BOG	A	912	-	20,20,20	0.59	0	25,25,25	1.24	3 (12%)
9	A1H1T	A	901	-	54,57,57	2.14	11 (20%)	57,70,70	1.56	12 (21%)
6	C8E	A	910	-	9,9,20	0.40	0	8,8,19	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	909	-	3,3,3	0.84	0	3,3,3	0.62	0
2	BOG	A	908	-	20,20,20	0.45	0	25,25,25	0.62	0
2	BOG	A	902	-	20,20,20	0.45	0	25,25,25	0.49	0
3	GOL	A	905	-	5,5,5	0.24	0	5,5,5	0.40	0
7	SO4	A	917	-	4,4,4	0.56	0	6,6,6	0.18	0
7	SO4	A	916	-	4,4,4	0.63	0	6,6,6	0.35	0
3	GOL	A	904	-	5,5,5	0.32	0	5,5,5	0.36	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
6	C8E	A	913	-	-	12/18/18/18	-
2	BOG	A	903	-	-	4/6/6/31	-
6	C8E	A	911	-	-	5/7/7/18	-
3	GOL	A	914	-	-	4/4/4/4	-
9	A1H1T	A	901	-	-	27/60/63/63	0/2/2/2
2	BOG	A	912	-	-	9/11/31/31	0/1/1/1
6	C8E	A	910	-	-	4/7/7/18	-
2	BOG	A	908	-	-	8/11/31/31	0/1/1/1
2	BOG	A	902	-	-	8/11/31/31	0/1/1/1
3	GOL	A	905	-	-	2/4/4/4	-
3	GOL	A	904	-	-	4/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	901	A1H1T	C14-N03	7.57	1.45	1.35
9	A	901	A1H1T	C05-N01	7.11	1.45	1.35
9	A	901	A1H1T	C17-N04	5.39	1.46	1.33
9	A	901	A1H1T	C25-N06	5.03	1.45	1.33
9	A	901	A1H1T	C08-N02	5.00	1.45	1.33
9	A	901	A1H1T	O05-C08	-2.75	1.17	1.23
9	A	901	A1H1T	O06-C14	-2.57	1.17	1.23
9	A	901	A1H1T	O01-C25	-2.51	1.18	1.23
9	A	901	A1H1T	O03-C17	-2.44	1.18	1.23
9	A	901	A1H1T	O02-C05	-2.37	1.17	1.23
9	A	901	A1H1T	C29-N07	2.04	1.44	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	912	BOG	O5-C1-C2	3.89	118.36	110.37
9	A	901	A1H1T	C29-N07-C28	-3.58	116.38	122.44
9	A	901	A1H1T	C37-N09-C29	3.52	121.92	116.81
9	A	901	A1H1T	C30-N08-C28	3.45	121.82	116.81
2	A	912	BOG	C1-O5-C5	2.81	119.20	113.72
9	A	901	A1H1T	C16-C17-N04	2.68	121.22	116.34
2	A	912	BOG	C1-C2-C3	2.63	115.54	110.01
9	A	901	A1H1T	C26-C25-N06	2.62	121.36	115.64
9	A	901	A1H1T	C15-C16-C17	2.57	117.94	112.67
9	A	901	A1H1T	C31-C30-N08	-2.45	119.54	123.42
9	A	901	A1H1T	C03-C04-N01	-2.35	106.12	110.94
9	A	901	A1H1T	C36-C35-C34	-2.28	117.42	120.24
9	A	901	A1H1T	C07-C08-N02	2.28	120.50	116.34
9	A	901	A1H1T	O08-N03-C13	2.00	118.45	113.76
9	A	901	A1H1T	O01-C25-N06	-2.00	119.10	123.03

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	902	BOG	O5-C1-O1-C1'
2	A	912	BOG	C2-C1-O1-C1'
2	A	912	BOG	O5-C1-O1-C1'
2	A	912	BOG	C2'-C1'-O1-C1
3	A	904	GOL	O1-C1-C2-C3
3	A	904	GOL	C1-C2-C3-O3
9	A	901	A1H1T	C14-C15-C16-C17
9	A	901	A1H1T	C12-C13-N03-O08
9	A	901	A1H1T	C02-C03-C04-N01
9	A	901	A1H1T	C34-C29-N07-C28
9	A	901	A1H1T	N09-C29-N07-C28
6	A	913	C8E	C17-C16-O15-C14
9	A	901	A1H1T	C16-C17-N04-C18
9	A	901	A1H1T	C07-C08-N02-C09
9	A	901	A1H1T	C24-C01-C02-C03
2	A	908	BOG	O5-C1-O1-C1'
9	A	901	A1H1T	O03-C17-N04-C18
9	A	901	A1H1T	O01-C25-N06-C24
9	A	901	A1H1T	O05-C08-N02-C09
2	A	908	BOG	O5-C5-C6-O6
9	A	901	A1H1T	C02-C01-C24-N06

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Mol	Chain	Res	Type	Atoms
2	A	908	BOG	C4-C5-C6-O6
2	A	908	BOG	C2-C1-O1-C1'
3	A	904	GOL	O1-C1-C2-O2
9	A	901	A1H1T	C26-C25-N06-C24
6	A	910	C8E	C7-C8-O9-C10
6	A	911	C8E	C7-C8-O9-C10
6	A	913	C8E	O18-C19-C20-O21
6	A	913	C8E	O9-C10-C11-O12
2	A	912	BOG	O1-C1'-C2'-C3'
3	A	914	GOL	O1-C1-C2-C3
3	A	904	GOL	O2-C2-C3-O3
2	A	908	BOG	C3'-C4'-C5'-C6'
6	A	911	C8E	C3-C4-C5-C6
6	A	913	C8E	C1-C2-C3-C4
2	A	903	BOG	C2'-C3'-C4'-C5'
2	A	903	BOG	C4'-C5'-C6'-C7'
6	A	913	C8E	C4-C5-C6-C7
9	A	901	A1H1T	C10-C11-C12-C13
9	A	901	A1H1T	C19-C20-C21-C22
2	A	902	BOG	C4'-C5'-C6'-C7'
2	A	902	BOG	C3'-C4'-C5'-C6'
2	A	908	BOG	C2'-C3'-C4'-C5'
6	A	911	C8E	C2-C3-C4-C5
2	A	902	BOG	O5-C5-C6-O6
2	A	903	BOG	C1'-C2'-C3'-C4'
6	A	911	C8E	C5-C6-C7-C8
9	A	901	A1H1T	N09-C29-N07-C26
2	A	912	BOG	O5-C5-C6-O6
6	A	910	C8E	C2-C3-C4-C5
2	A	902	BOG	C4-C5-C6-O6
2	A	902	BOG	C5'-C6'-C7'-C8'
3	A	914	GOL	O1-C1-C2-O2
6	A	913	C8E	C2-C3-C4-C5
9	A	901	A1H1T	C01-C02-C03-C04
2	A	912	BOG	C5'-C6'-C7'-C8'
2	A	902	BOG	C2'-C3'-C4'-C5'
6	A	913	C8E	O15-C16-C17-O18
9	A	901	A1H1T	C12-C13-N03-C14
9	A	901	A1H1T	N03-C14-C15-C16
2	A	912	BOG	C4'-C5'-C6'-C7'
6	A	910	C8E	C3-C4-C5-C6
2	A	908	BOG	O1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
2	A	902	BOG	C2'-C1'-O1-C1
6	A	913	C8E	C16-C17-O18-C19
6	A	910	C8E	C1-C2-C3-C4
6	A	913	C8E	C20-C19-O18-C17
9	A	901	A1H1T	O02-C05-N01-O07
6	A	913	C8E	C5-C6-C7-C8
9	A	901	A1H1T	C34-C29-N07-C26
6	A	911	C8E	C4-C5-C6-C7
3	A	905	GOL	O1-C1-C2-C3
3	A	914	GOL	C1-C2-C3-O3
3	A	914	GOL	O2-C2-C3-O3
6	A	913	C8E	C7-C8-O9-C10
9	A	901	A1H1T	C05-C06-C07-C08
9	A	901	A1H1T	O06-C14-C15-C16
2	A	903	BOG	C3'-C4'-C5'-C6'
2	A	912	BOG	C2'-C3'-C4'-C5'
2	A	908	BOG	C2'-C1'-O1-C1
9	A	901	A1H1T	C27-C23-N05-O09
2	A	912	BOG	C3'-C4'-C5'-C6'
9	A	901	A1H1T	N01-C05-C06-C07
6	A	913	C8E	C10-C11-O12-C13
9	A	901	A1H1T	O04-C23-N05-O09
9	A	901	A1H1T	O06-C14-N03-O08
3	A	905	GOL	O1-C1-C2-O2

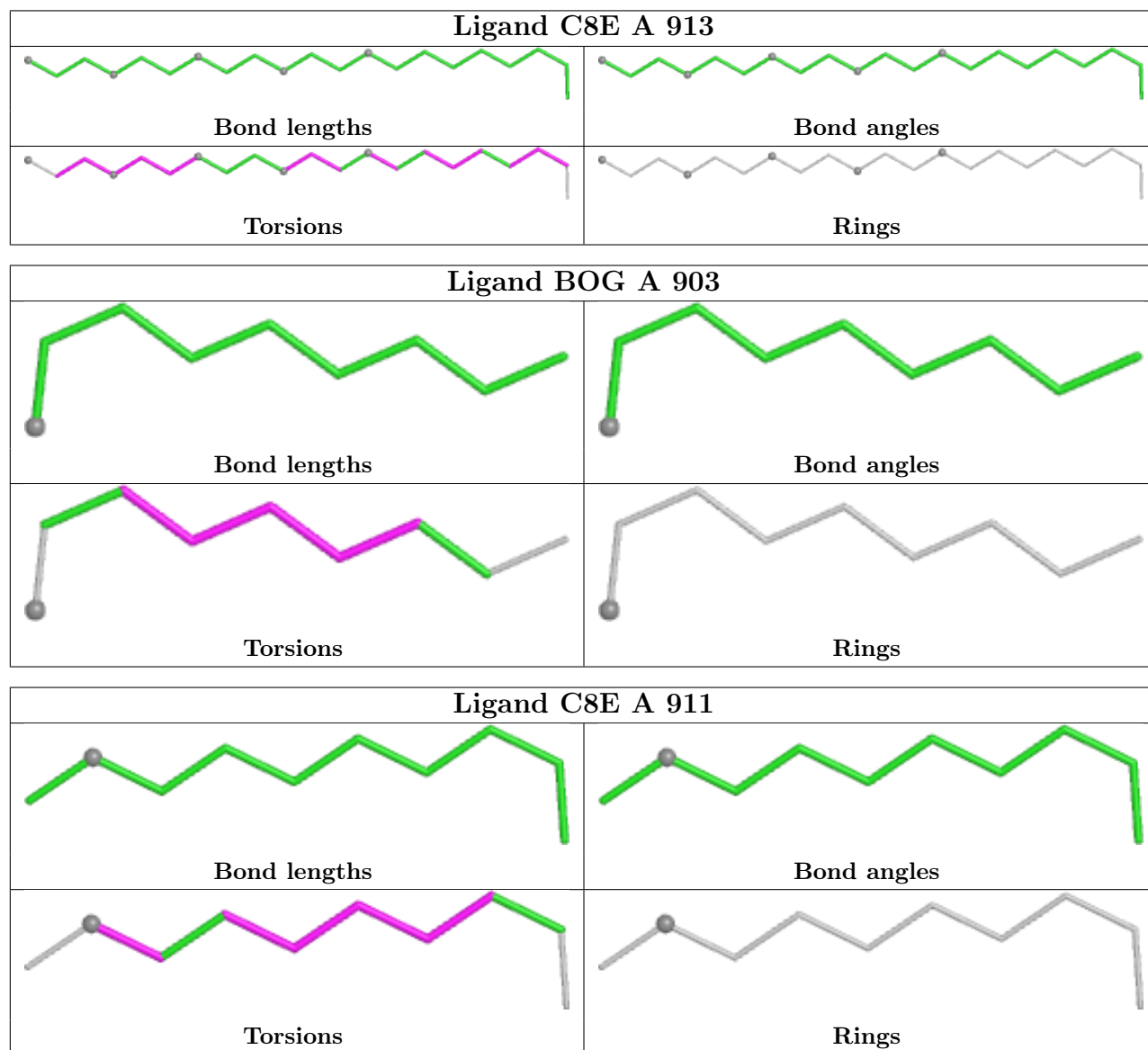
There are no ring outliers.

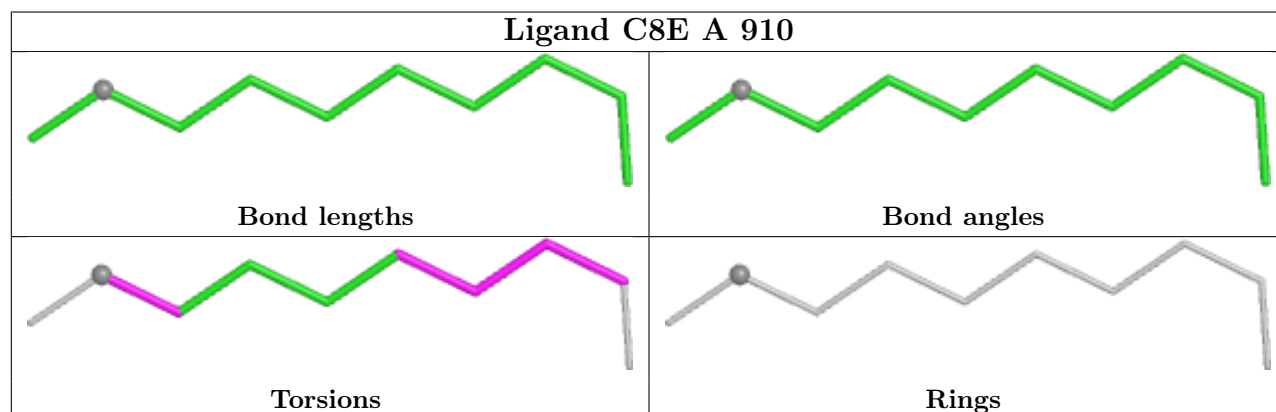
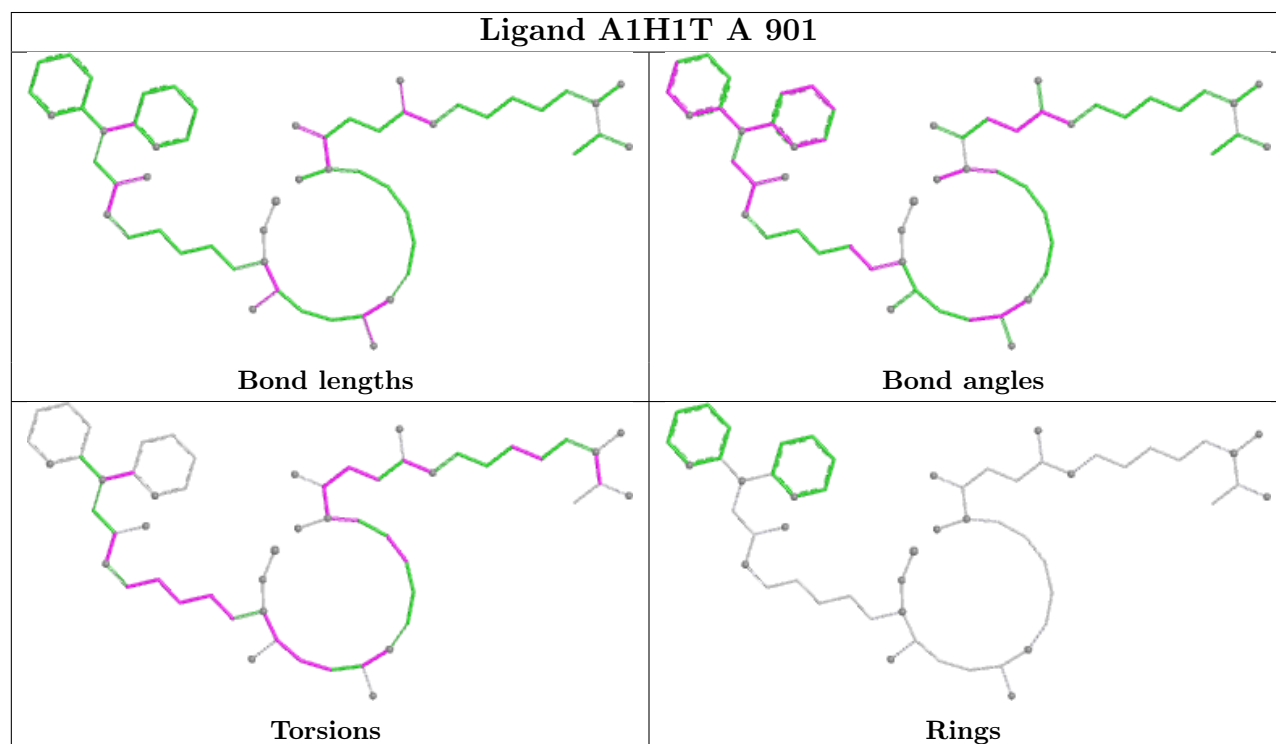
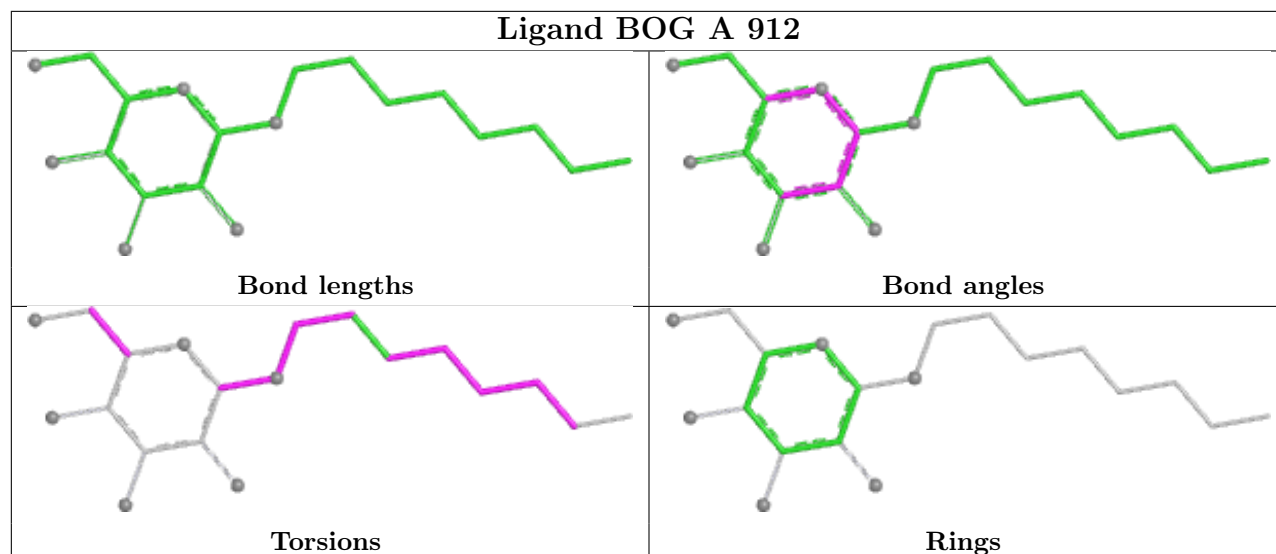
4 monomers are involved in 8 short contacts:

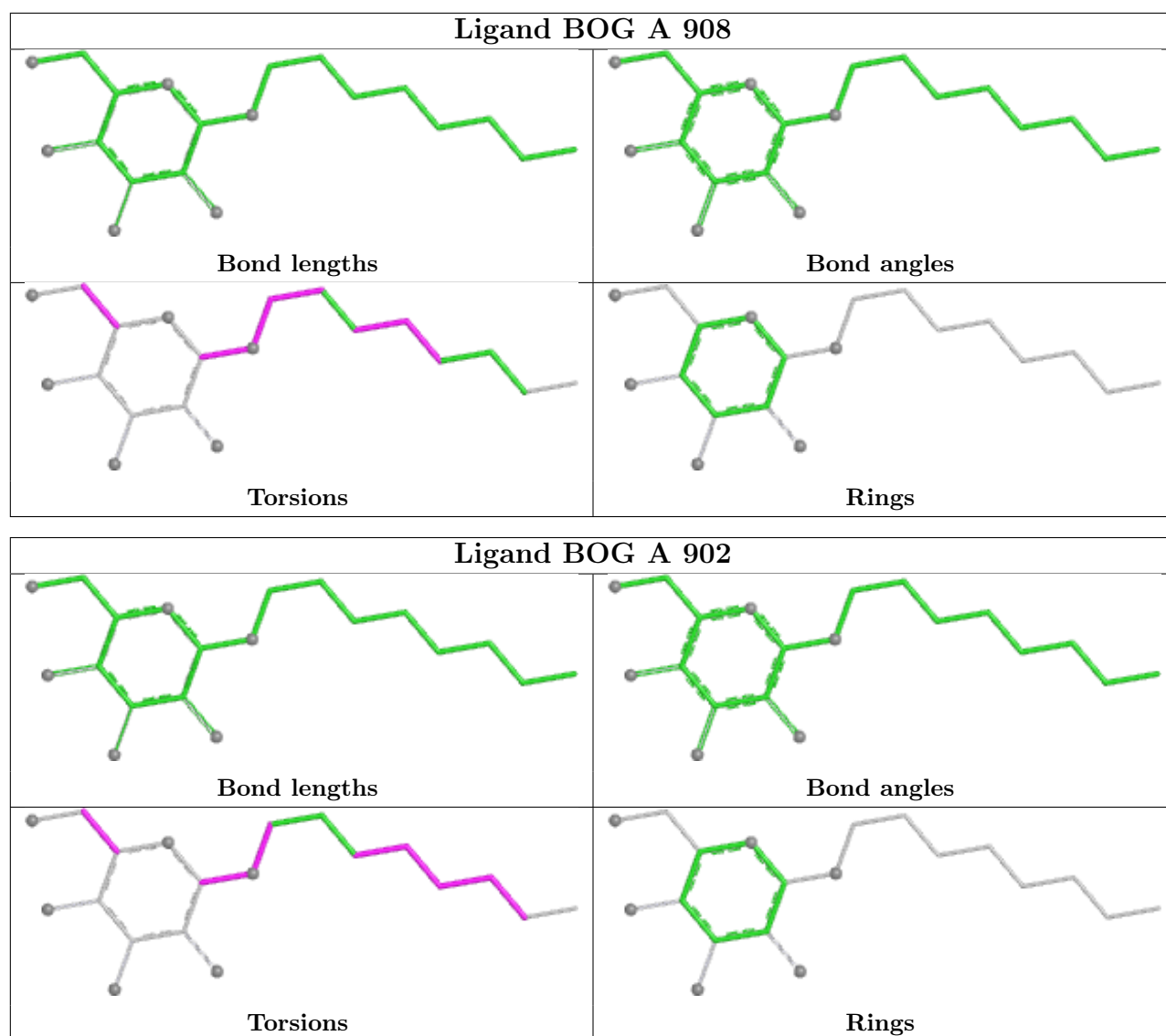
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	913	C8E	2	0
3	A	914	GOL	1	0
5	A	909	DMS	4	0
2	A	902	BOG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	677/820 (82%)	0.56	57 (8%) 17 15	38, 55, 90, 125	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	398	GLY	5.5
1	A	614	ALA	5.4
1	A	391	ILE	4.5
1	A	389	ARG	4.2
1	A	144	VAL	4.2
1	A	613	ASP	4.2
1	A	730	ALA	4.0
1	A	732	PRO	4.0
1	A	663	PHE	4.0
1	A	731	GLY	3.8
1	A	395	PHE	3.7
1	A	393	ARG	3.6
1	A	683	LEU	3.5
1	A	396	PHE	3.5
1	A	611	TYR	3.3
1	A	200	ARG	3.2
1	A	582	PHE	3.1
1	A	445	TYR	3.0
1	A	637	GLY	3.0
1	A	412	PHE	2.9
1	A	684	SER	2.9
1	A	818	TYR	2.9
1	A	705	ASP	2.8
1	A	615	SER	2.8
1	A	449	ALA	2.8
1	A	646	LEU	2.8
1	A	820	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	298	ILE	2.6
1	A	446	GLY	2.6
1	A	780	LEU	2.6
1	A	145	PHE	2.6
1	A	777	LEU	2.5
1	A	421	ASP	2.5
1	A	400	PRO	2.5
1	A	514	PHE	2.4
1	A	733	LEU	2.4
1	A	752	LYS	2.3
1	A	635	ALA	2.3
1	A	515	ASN	2.2
1	A	617	THR	2.2
1	A	728	PHE	2.2
1	A	754	ASN	2.2
1	A	469	TYR	2.2
1	A	662	ASN	2.1
1	A	333	THR	2.1
1	A	664	TYR	2.1
1	A	690	LEU	2.1
1	A	517	VAL	2.1
1	A	579	TRP	2.1
1	A	659	PRO	2.1
1	A	450	SER	2.1
1	A	338	VAL	2.1
1	A	806	PHE	2.1
1	A	317	GLU	2.1
1	A	753	GLU	2.1
1	A	810	ARG	2.1
1	A	226	ASP	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

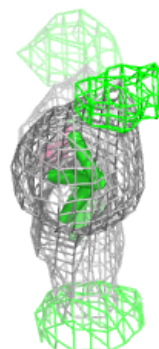
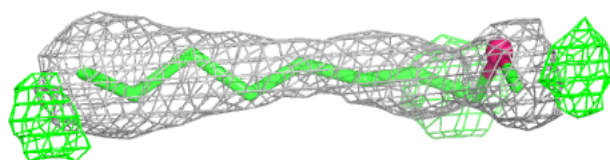
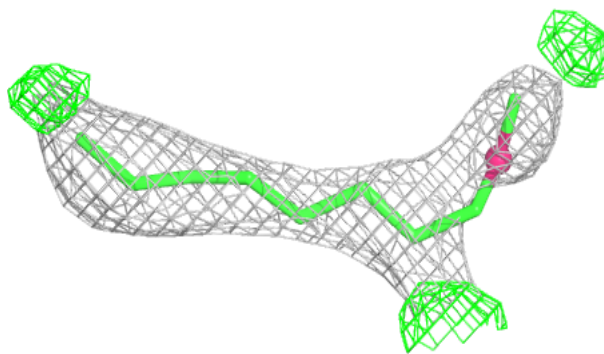
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NH4	A	907	1/1	0.70	0.28	50,50,50,50	0
6	C8E	A	910	10/21	0.70	0.28	60,63,72,73	0
2	BOG	A	908	20/20	0.72	0.21	65,70,78,78	0
2	BOG	A	902	20/20	0.73	0.20	68,73,78,79	0
3	GOL	A	904	6/6	0.78	0.16	54,55,56,56	0
2	BOG	A	912	20/20	0.79	0.19	77,86,94,96	0
3	GOL	A	905	6/6	0.82	0.18	66,67,68,69	0
3	GOL	A	914	6/6	0.82	0.15	48,50,54,54	0
6	C8E	A	913	21/21	0.83	0.18	65,71,83,84	0
4	NH4	A	906	1/1	0.85	0.26	54,54,54,54	0
7	SO4	A	918	5/5	0.85	0.20	48,49,52,55	0
9	A1H1T	A	901	56/56	0.85	0.20	42,57,67,68	0
7	SO4	A	917	5/5	0.86	0.20	51,52,55,57	0
6	C8E	A	911	10/21	0.86	0.22	69,72,78,79	0
5	DMS	A	909	4/4	0.86	0.20	52,58,59,59	0
7	SO4	A	916	5/5	0.87	0.16	48,52,55,56	0
2	BOG	A	903	9/20	0.88	0.15	57,58,63,65	0
8	NA	A	919	1/1	0.94	0.18	51,51,51,51	0

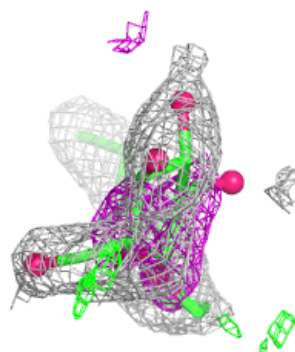
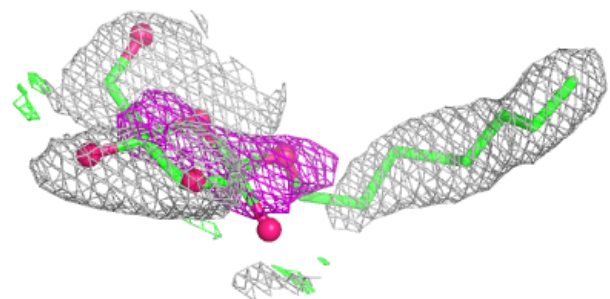
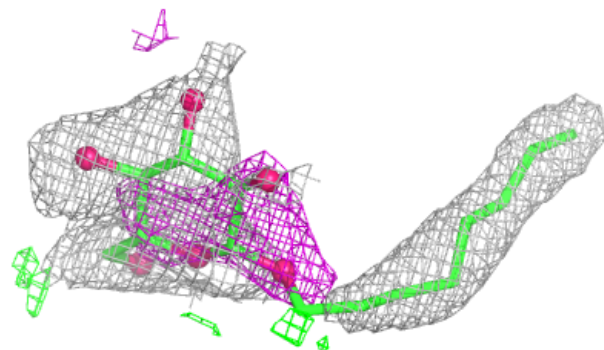
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E A 910:

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

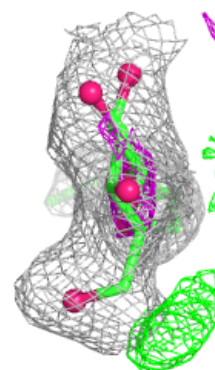
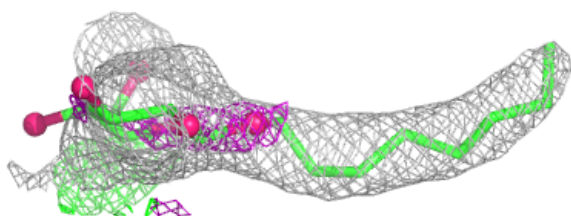
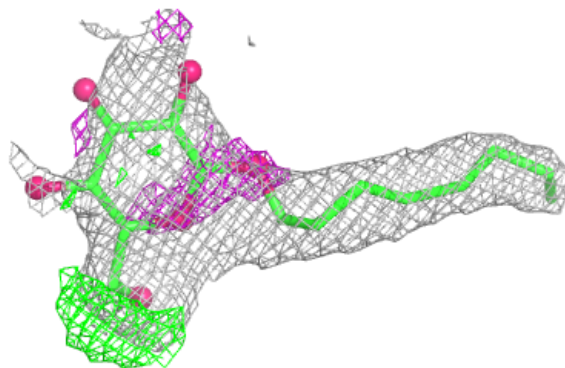
**Electron density around BOG A 908:**

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

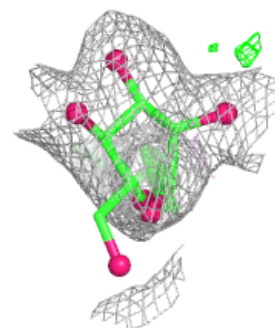
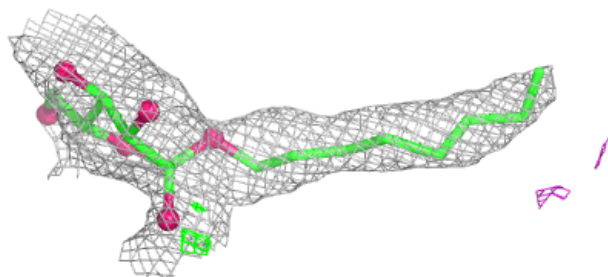
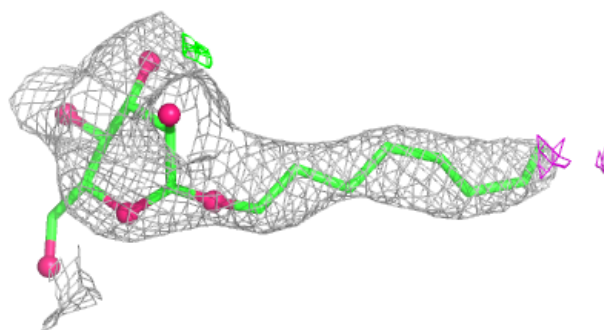


Electron density around BOG A 902:

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

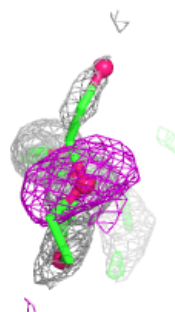
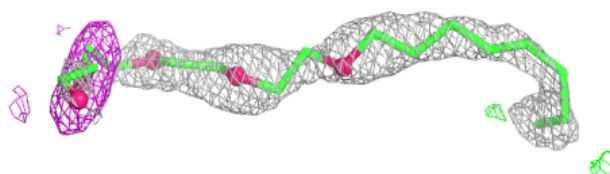
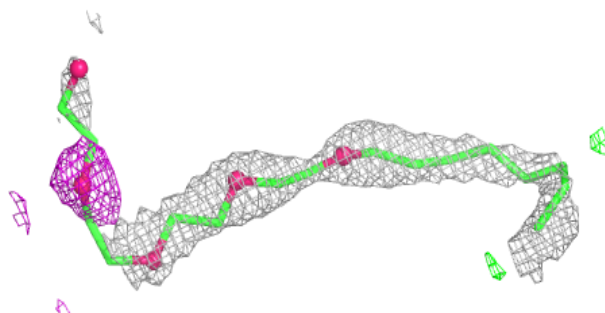
**Electron density around BOG A 912:**

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



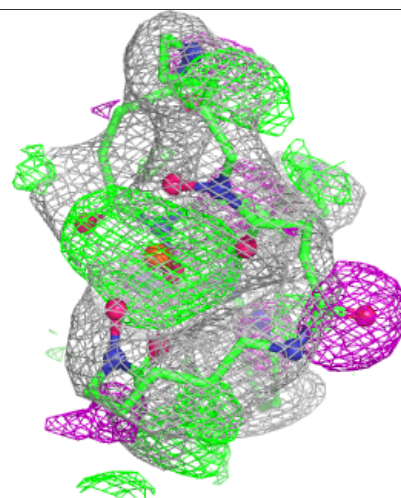
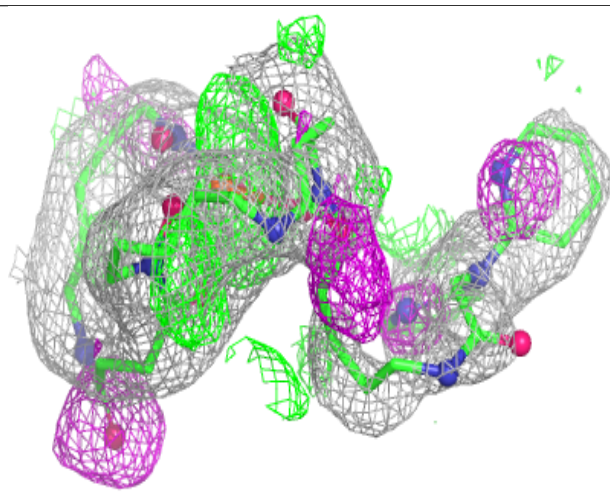
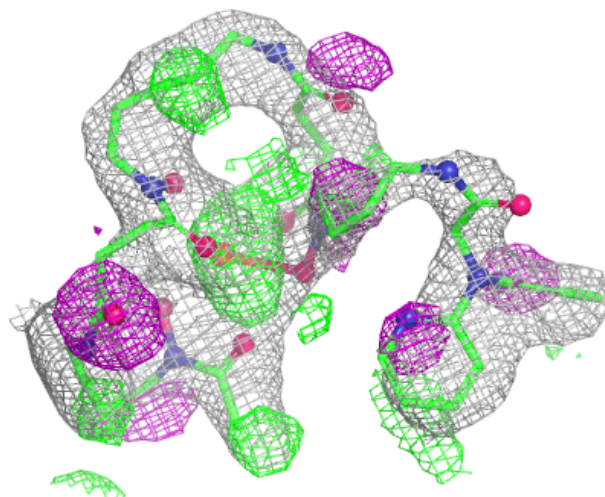
Electron density around C8E A 913:

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



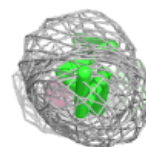
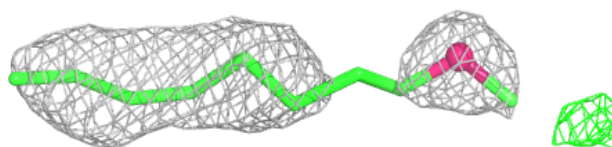
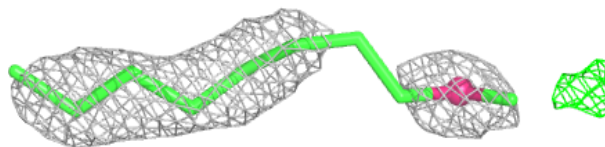
Electron density around A1H1T A 901:

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

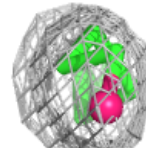
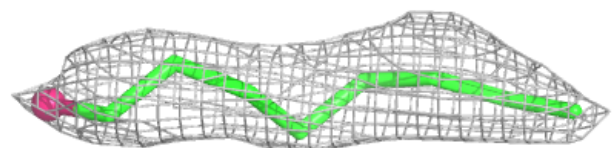
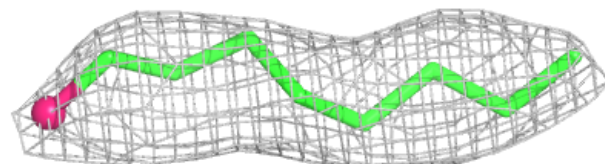


Electron density around C8E A 911:

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

**Electron density around BOG A 903:**

$2mF_o-DF_c$ (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.