Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 09:47 AM EDT

PDB ID	:	6I96
Title	:	Structure of the ferrioxamine B transporter FoxA from Pseudomonas aeruginosa in complex with ferrioxamine B
Authors	:	Josts, I.; Tidow, H.
Deposited on	:	2018-11-22
Resolution	:	1.85 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:

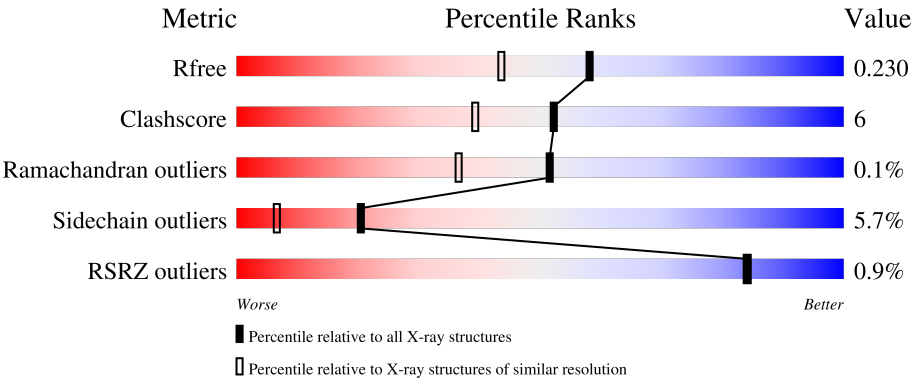
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 <=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	677	% 82% 14%

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
2	0UE	A	901	X	-	-	-

2 Entry composition

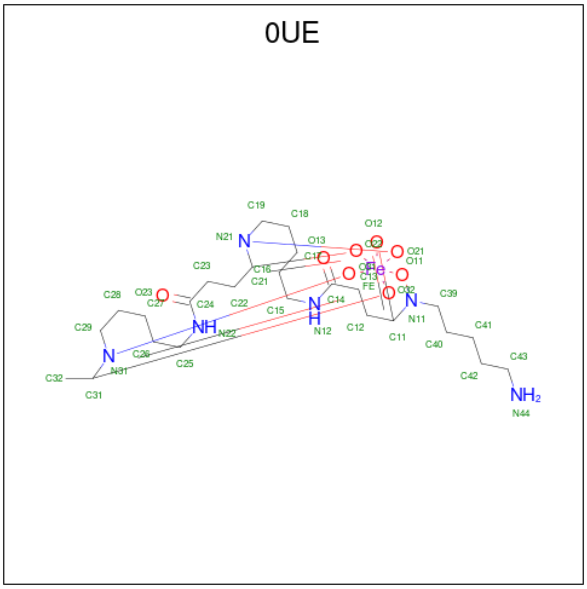
There are 7 unique types of molecules in this entry. The entry contains 5945 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ferric hydroxamate uptake.

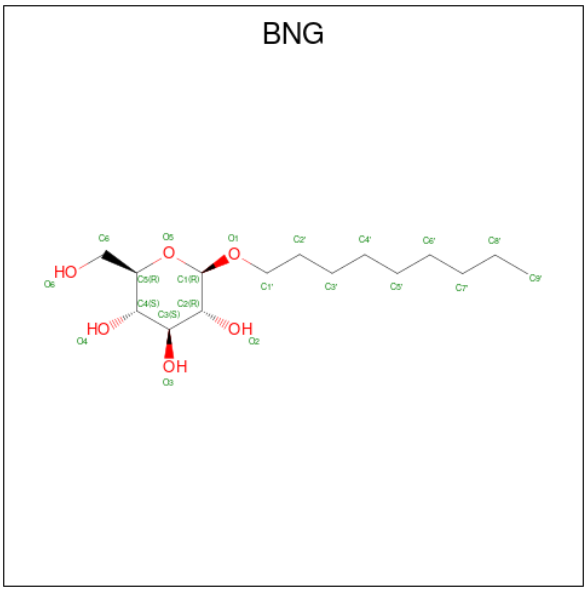
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	677	Total	C	N	O	S	0	0	0
			5325	3345	910	1059	11			

- Molecule 2 is Ferrioxamine B (three-letter code: 0UE) (formula: $C_{25}H_{45}FeN_6O_8$).



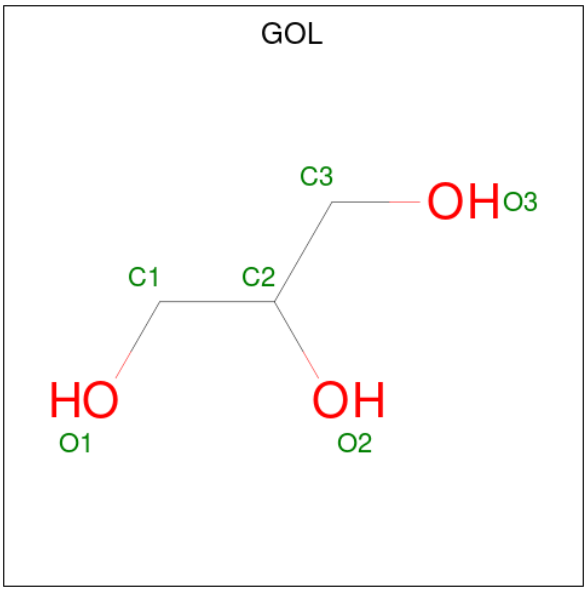
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			40	25	1	6	8		

- Molecule 3 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).



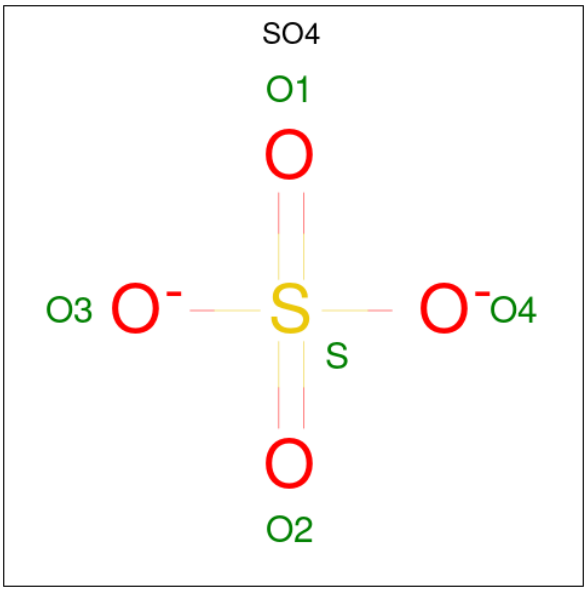
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 10 2	0	0
3	A	1	Total C O 21 15 6	0	0
3	A	1	Total C O 21 15 6	0	0
3	A	1	Total C O 21 15 6	0	0
3	A	1	Total C O 21 15 6	0	0
3	A	1	Total C O 21 15 6	0	0
3	A	1	Total C O 21 15 6	0	0
3	A	1	Total C O 21 15 6	0	0
3	A	1	Total C O 10 9 1	0	0
3	A	1	Total C O 21 15 6	0	0
3	A	1	Total C O 21 15 6	0	0
3	A	1	Total C O 21 15 6	0	0
3	A	1	Total C O 21 15 6	0	0

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



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Na 2 2	0	0

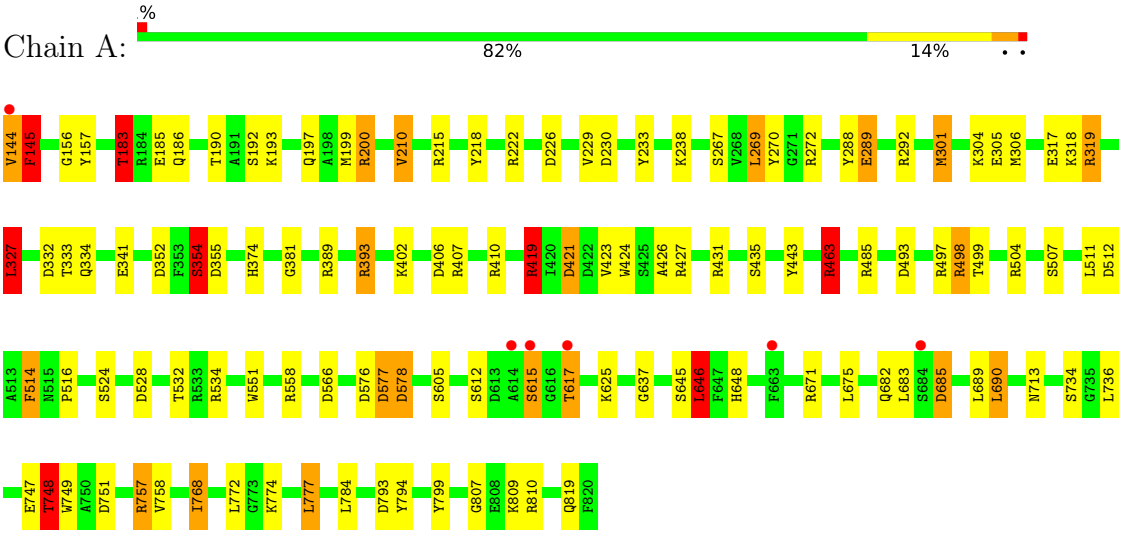
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	257	Total O 257 257	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ferric hydroxamate uptake



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	94.89Å 94.89Å 177.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.18 – 1.85 82.18 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (82.18-1.85) 99.2 (82.18-1.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.181 , 0.219 0.191 , 0.230	Depositor DCC
R_{free} test set	3949 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5945	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, 0UE, SO4, BNG, 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	1.36	21/5451 (0.4%)	1.34	57/7397 (0.8%)

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	3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	ASP	CB-CG	-8.78	1.33	1.51
1	A	671	ARG	CZ-NH1	7.88	1.43	1.33
1	A	333	THR	N-CA	7.78	1.61	1.46
1	A	524	SER	CB-OG	-7.68	1.32	1.42
1	A	145	PHE	CE1-CZ	7.18	1.50	1.37
1	A	748	THR	CB-CG2	-6.93	1.29	1.52
1	A	498	ARG	CZ-NH2	6.89	1.42	1.33
1	A	341	GLU	CD-OE1	6.47	1.32	1.25
1	A	749	TRP	CE3-CZ3	6.45	1.49	1.38
1	A	435	SER	CB-OG	-6.20	1.34	1.42
1	A	421	ASP	CA-CB	6.10	1.67	1.53
1	A	354	SER	C-O	5.58	1.33	1.23
1	A	289	GLU	CG-CD	5.43	1.60	1.51
1	A	145	PHE	CE2-CZ	5.33	1.47	1.37
1	A	183	THR	CB-CG2	-5.24	1.35	1.52
1	A	551	TRP	CE3-CZ3	5.14	1.47	1.38
1	A	230	ASP	CB-CG	5.12	1.62	1.51
1	A	645	SER	CA-CB	5.11	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	VAL	CB-CG1	-5.04	1.42	1.52
1	A	751	ASP	CB-CG	5.02	1.62	1.51
1	A	566	ASP	CB-CG	5.01	1.62	1.51

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	421	ASP	CB-CG-OD1	-27.14	93.87	118.30
1	A	421	ASP	CB-CG-OD2	19.82	136.13	118.30
1	A	410	ARG	NE-CZ-NH1	13.91	127.25	120.30
1	A	671	ARG	NE-CZ-NH2	-12.74	113.93	120.30
1	A	810	ARG	NE-CZ-NH2	-12.48	114.06	120.30
1	A	419	ARG	NE-CZ-NH2	10.29	125.45	120.30
1	A	199	MET	CG-SD-CE	-9.98	84.23	100.20
1	A	410	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	A	810	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	393	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	A	332	ASP	C-N-CA	-8.47	100.52	121.70
1	A	200	ARG	NE-CZ-NH1	-8.28	116.16	120.30
1	A	319	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	463	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	504	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	292	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	A	463	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	292	ARG	NE-CZ-NH1	-7.27	116.67	120.30
1	A	352	ASP	CB-CG-OD1	7.22	124.79	118.30
1	A	504	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	301	MET	CG-SD-CE	6.93	111.28	100.20
1	A	751	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	419	ARG	CD-NE-CZ	6.84	133.17	123.60
1	A	793	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	528	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	226	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	427	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	757	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	747	GLU	OE1-CD-OE2	6.33	130.90	123.30
1	A	327	LEU	CB-CG-CD1	-6.22	100.42	111.00
1	A	685	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	497	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	222	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	431	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	748	THR	N-CA-CB	-5.89	99.11	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	671	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	646	LEU	CA-CB-CG	5.77	128.57	115.30
1	A	498	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	493	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	272	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	646	LEU	CB-CG-CD1	5.62	120.56	111.00
1	A	327	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	222	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	269	LEU	CB-CG-CD1	5.42	120.21	111.00
1	A	210	VAL	CG1-CB-CG2	-5.37	102.32	110.90
1	A	332	ASP	O-C-N	-5.35	114.14	122.70
1	A	215	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	183	THR	N-CA-CB	-5.26	100.30	110.30
1	A	407	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	507	SER	CA-CB-OG	-5.14	97.31	111.20
1	A	381	GLY	N-CA-C	5.10	125.85	113.10
1	A	332	ASP	N-CA-C	-5.09	97.27	111.00
1	A	200	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	406	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	270	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	A	690	LEU	CA-CB-CG	5.04	126.88	115.30
1	A	558	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	VAL	Peptide
1	A	145	PHE	Mainchain
1	A	637	GLY	Peptide

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	5325	0	5038	53	0
2	A	40	0	41	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	253	0	368	7	0
4	A	48	0	64	1	0
5	A	20	0	0	0	0
6	A	2	0	0	0	0
7	A	257	0	0	6	0
All	All	5945	0	5511	62	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 (62) 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)
2:A:901:0UE:N31	2:A:901:0UE:C31	1.70	1.51
2:A:901:0UE:C21	2:A:901:0UE:N21	1.81	1.44
2:A:901:0UE:N11	2:A:901:0UE:C11	1.85	1.39
1:A:757:ARG:HH22	3:A:913:BNG:H2	1.39	0.86
2:A:901:0UE:C21	2:A:901:0UE:C19	2.52	0.85
1:A:183:THR:HG22	1:A:186:GLN:H	1.52	0.74
1:A:301:MET:CE	1:A:334:GLN:HB3	2.19	0.72
2:A:901:0UE:C21	2:A:901:0UE:O21	2.37	0.71
1:A:157:TYR:H	1:A:682:GLN:HE22	1.37	0.71
2:A:901:0UE:C11	2:A:901:0UE:C39	2.61	0.69
1:A:421:ASP:HB3	1:A:423:VAL:H	1.58	0.67
1:A:197:GLN:O	1:A:200:ARG:NE	2.29	0.65
1:A:736:LEU:HD11	1:A:768:ILE:HD11	1.79	0.65
1:A:218:TYR:HE1	2:A:901:0UE:H8	1.62	0.64
1:A:485:ARG:NH2	7:A:1003:HOH:O	2.31	0.62
1:A:301:MET:HE2	1:A:334:GLN:HB3	1.82	0.61
1:A:301:MET:HE3	1:A:809:LYS:HG2	1.83	0.60
1:A:534:ARG:NH1	3:A:906:BNG:O2	2.36	0.59
1:A:156:GLY:O	1:A:183:THR:HG21	2.04	0.58
1:A:757:ARG:NH2	3:A:913:BNG:H2	2.14	0.56
1:A:183:THR:HB	7:A:1073:HOH:O	2.05	0.55
1:A:443:TYR:CE2	2:A:901:0UE:H29	2.42	0.55
1:A:734:SER:HB3	1:A:774:LYS:HE2	1.90	0.54
1:A:218:TYR:OH	1:A:374:HIS:HE1	1.93	0.52
3:A:911:BNG:HO3	3:A:911:BNG:HO6	1.56	0.51
1:A:736:LEU:CD1	1:A:768:ILE:HD11	2.39	0.50
1:A:421:ASP:HB2	1:A:424:TRP:H	1.77	0.49
1:A:419:ARG:NH2	7:A:1010:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:LEU:HD13	1:A:675:LEU:HD13	1.94	0.49
1:A:615:SER:HB2	1:A:617:THR:HG22	1.95	0.49
1:A:772:LEU:HB3	1:A:777:LEU:HD11	1.95	0.49
1:A:426:ALA:HB1	3:A:904:BNG:H1	1.94	0.48
1:A:301:MET:HE1	1:A:334:GLN:N	2.28	0.48
1:A:576:ASP:C	1:A:577:ASP:OD1	2.52	0.48
1:A:419:ARG:HH21	1:A:419:ARG:HG3	1.79	0.47
1:A:498:ARG:HD2	3:A:906:BNG:H1	1.97	0.47
1:A:648:HIS:HD2	7:A:1232:HOH:O	1.98	0.47
1:A:301:MET:CE	1:A:809:LYS:HG2	2.45	0.47
1:A:532:THR:OG1	4:A:920:GOL:H31	2.14	0.47
1:A:794:TYR:CZ	1:A:807:GLY:HA3	2.50	0.47
1:A:192:SER:OG	1:A:200:ARG:NH1	2.47	0.46
1:A:748:THR:CG2	7:A:1180:HOH:O	2.63	0.46
1:A:463:ARG:HD2	7:A:1096:HOH:O	2.16	0.46
1:A:512:ASP:OD1	1:A:514:PHE:O	2.34	0.46
1:A:233:TYR:CZ	1:A:238:LYS:HD3	2.51	0.46
2:A:901:0UE:C31	2:A:901:0UE:C29	2.82	0.46
1:A:305:GLU:OE1	1:A:327:LEU:HD13	2.15	0.46
1:A:218:TYR:OH	1:A:374:HIS:CE1	2.70	0.45
2:A:901:0UE:N21	2:A:901:0UE:C22	2.64	0.44
1:A:183:THR:HG23	1:A:185:GLU:H	1.83	0.43
1:A:190:THR:CB	1:A:200:ARG:HH12	2.31	0.43
1:A:578:ASP:HB3	3:A:905:BNG:H3	2.00	0.43
1:A:713:ASN:ND2	1:A:799:TYR:O	2.52	0.43
1:A:288:TYR:O	1:A:318:LYS:HE3	2.18	0.43
1:A:267:SER:HB2	1:A:605:SER:HA	2.01	0.43
1:A:511:LEU:HD11	1:A:516:PRO:HB2	2.01	0.43
1:A:210:VAL:HG12	1:A:210:VAL:O	2.20	0.42
1:A:319:ARG:HH12	1:A:354:SER:HA	1.83	0.42
1:A:748:THR:HG22	1:A:758:VAL:HB	2.01	0.42
1:A:157:TYR:CB	1:A:690:LEU:HD21	2.49	0.42
1:A:576:ASP:C	1:A:577:ASP:CG	2.77	0.40
1:A:768:ILE:HG23	1:A:784:LEU:HB3	2.02	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	675/677 (100%)	652 (97%)	22 (3%)	1 (0%)	51 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	PHE

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	566/566 (100%)	534 (94%)	32 (6%)	20 6

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	VAL
1	A	183	THR
1	A	193	LYS
1	A	269	LEU
1	A	289	GLU
1	A	304	LYS
1	A	306	MET
1	A	317	GLU
1	A	327	LEU
1	A	354	SER

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Mol	Chain	Res	Type
1	A	355	ASP
1	A	389	ARG
1	A	393	ARG
1	A	402	LYS
1	A	419	ARG
1	A	463	ARG
1	A	499	THR
1	A	514	PHE
1	A	577	ASP
1	A	578	ASP
1	A	612	SER
1	A	615	SER
1	A	617	THR
1	A	625	LYS
1	A	646	LEU
1	A	683	LEU
1	A	685	ASP
1	A	689	LEU
1	A	748	THR
1	A	768	ILE
1	A	777	LEU
1	A	819	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	374	HIS
1	A	385	HIS
1	A	387	ASN
1	A	390	HIS
1	A	653	ASN
1	A	682	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
3	BNG	A	905	-	21,21,21	0.98	1 (4%)	26,26,26	1.81	6 (23%)
3	BNG	A	910	-	9,9,21	0.28	0	8,8,26	0.73	0
5	SO4	A	923	-	4,4,4	0.59	0	6,6,6	0.48	0
3	BNG	A	909	-	21,21,21	0.86	1 (4%)	26,26,26	1.30	3 (11%)
3	BNG	A	904	-	21,21,21	0.67	0	26,26,26	1.11	1 (3%)
3	BNG	A	903	-	21,21,21	0.98	1 (4%)	26,26,26	1.62	3 (11%)
4	GOL	A	916	-	5,5,5	0.64	0	5,5,5	1.51	0
4	GOL	A	921	-	5,5,5	0.85	0	5,5,5	1.62	2 (40%)
3	BNG	A	902	-	11,11,21	0.57	0	9,10,26	0.21	0
3	BNG	A	911	-	21,21,21	1.12	1 (4%)	26,26,26	1.44	3 (11%)
3	BNG	A	907	-	21,21,21	0.71	1 (4%)	26,26,26	1.48	4 (15%)
4	GOL	A	915	-	5,5,5	0.39	0	5,5,5	0.81	0
3	BNG	A	908	-	21,21,21	0.62	0	26,26,26	0.99	2 (7%)
3	BNG	A	906	-	21,21,21	0.76	1 (4%)	26,26,26	1.51	4 (15%)
3	BNG	A	912	-	21,21,21	0.86	1 (4%)	26,26,26	1.36	4 (15%)
4	GOL	A	922	-	5,5,5	0.73	0	5,5,5	0.85	0
4	GOL	A	918	-	5,5,5	0.36	0	5,5,5	0.74	0
3	BNG	A	914	-	21,21,21	0.54	0	26,26,26	1.20	3 (11%)
5	SO4	A	925	-	4,4,4	0.59	0	6,6,6	0.34	0
2	0UE	A	901	-	44,44,44	10.11	26 (59%)	44,66,66	8.69	27 (61%)
4	GOL	A	920	-	5,5,5	1.05	0	5,5,5	0.88	0
4	GOL	A	917	-	5,5,5	0.24	0	5,5,5	0.65	0
3	BNG	A	913	-	21,21,21	1.45	3 (14%)	26,26,26	3.24	7 (26%)
5	SO4	A	924	-	4,4,4	1.31	1 (25%)	6,6,6	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SO4	A	926	-	4,4,4	0.43	0	6,6,6	0.38	0
4	GOL	A	919	-	5,5,5	0.27	0	5,5,5	0.55	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	BNG	A	905	-	-	7/12/32/32	0/1/1/1
3	BNG	A	910	-	-	3/7/7/32	-
3	BNG	A	909	-	-	6/12/32/32	0/1/1/1
3	BNG	A	904	-	-	8/12/32/32	0/1/1/1
3	BNG	A	903	-	-	5/12/32/32	0/1/1/1
4	GOL	A	916	-	-	3/4/4/4	-
4	GOL	A	921	-	-	0/4/4/4	-
3	BNG	A	902	-	-	3/8/9/32	-
3	BNG	A	911	-	-	2/12/32/32	0/1/1/1
3	BNG	A	907	-	-	3/12/32/32	0/1/1/1
4	GOL	A	915	-	-	0/4/4/4	-
3	BNG	A	908	-	-	9/12/32/32	0/1/1/1
3	BNG	A	906	-	-	11/12/32/32	0/1/1/1
3	BNG	A	912	-	-	9/12/32/32	0/1/1/1
4	GOL	A	922	-	-	0/4/4/4	-
4	GOL	A	918	-	-	2/4/4/4	-
3	BNG	A	914	-	-	5/12/32/32	0/1/1/1
2	0UE	A	901	-	1/1/9/11	12/34/88/88	0/3/5/5
4	GOL	A	920	-	-	4/4/4/4	-
4	GOL	A	917	-	-	2/4/4/4	-
3	BNG	A	913	-	-	4/12/32/32	0/1/1/1
4	GOL	A	919	-	-	0/4/4/4	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	0UE	C11-N11	34.07	1.85	1.31
2	A	901	0UE	C21-N21	31.59	1.81	1.31
2	A	901	0UE	C39-N11	-25.61	1.02	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	0UE	C19-N21	-23.93	1.05	1.47
2	A	901	0UE	O22-C21	14.53	1.52	1.28
2	A	901	0UE	C31-N31	13.01	1.70	1.31
2	A	901	0UE	O32-C31	11.95	1.52	1.28
2	A	901	0UE	O31-N31	9.19	1.53	1.38
2	A	901	0UE	O11-N11	8.16	1.52	1.38
2	A	901	0UE	O12-C11	8.13	1.41	1.28
2	A	901	0UE	C12-C11	-7.74	1.29	1.51
2	A	901	0UE	C22-C21	-7.08	1.31	1.51
2	A	901	0UE	C24-N22	5.58	1.46	1.33
2	A	901	0UE	O21-FE	-5.54	1.86	1.99
2	A	901	0UE	O21-N21	5.44	1.47	1.38
2	A	901	0UE	O12-FE	-5.13	1.90	2.04
2	A	901	0UE	C23-C24	4.13	1.59	1.51
3	A	911	BNG	O1-C1	3.99	1.47	1.40
2	A	901	0UE	O22-FE	-3.96	1.93	2.04
2	A	901	0UE	C18-C19	3.85	1.67	1.51
3	A	913	BNG	O1-C1	3.79	1.46	1.40
3	A	913	BNG	C4-C3	-3.68	1.42	1.52
3	A	903	BNG	O1-C1	3.49	1.46	1.40
2	A	901	0UE	C15-N12	3.48	1.54	1.46
2	A	901	0UE	O32-FE	-3.27	1.95	2.04
2	A	901	0UE	C14-N12	3.25	1.40	1.33
3	A	905	BNG	O1-C1	3.17	1.45	1.40
3	A	912	BNG	O1-C1	3.04	1.45	1.40
2	A	901	0UE	O11-FE	-2.64	1.93	1.99
2	A	901	0UE	C17-C16	2.60	1.66	1.51
3	A	909	BNG	O1-C1	2.49	1.44	1.40
2	A	901	0UE	O23-C24	2.43	1.28	1.23
2	A	901	0UE	C17-C18	2.37	1.64	1.51
3	A	907	BNG	O1-C1	2.30	1.44	1.40
5	A	924	SO4	O2-S	2.16	1.57	1.46
3	A	913	BNG	C3-C2	-2.15	1.46	1.52
3	A	906	BNG	O1-C1	2.02	1.43	1.40

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	0UE	O21-N21-C21	-37.33	92.03	116.42
2	A	901	0UE	O11-N11-C11	-21.34	102.48	116.42
2	A	901	0UE	O22-C21-N21	-19.23	103.71	118.38
2	A	901	0UE	O22-C21-C22	16.72	137.74	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	0UE	O12-C11-N11	-13.95	107.73	118.38
3	A	913	BNG	O3-C3-C4	-9.40	88.63	110.35
3	A	913	BNG	O4-C4-C3	-8.77	90.06	110.35
2	A	901	0UE	O21-N21-C19	8.51	128.35	114.13
2	A	901	0UE	O11-N11-C39	7.79	127.15	114.13
2	A	901	0UE	C12-C11-N11	7.26	130.15	121.07
2	A	901	0UE	C13-C12-C11	6.45	118.51	112.27
3	A	913	BNG	O1-C1-C2	6.16	117.93	108.30
2	A	901	0UE	O32-C31-N31	-6.06	108.34	118.42
2	A	901	0UE	C19-N21-C21	-6.05	121.73	128.89
2	A	901	0UE	O31-N31-C29	5.64	123.56	114.13
2	A	901	0UE	C18-C19-N21	5.61	122.43	110.88
2	A	901	0UE	O32-C31-C32	5.60	130.29	119.49
2	A	901	0UE	C15-N12-C14	-5.55	112.53	122.84
2	A	901	0UE	C12-C13-C14	5.49	122.18	112.56
3	A	913	BNG	C1'-O1-C1	-5.40	104.88	113.84
2	A	901	0UE	C28-C29-N31	-5.09	100.39	110.88
3	A	903	BNG	O1-C1-C2	5.05	116.18	108.30
2	A	901	0UE	C22-C21-N21	-4.85	115.00	121.07
2	A	901	0UE	C23-C22-C21	-4.76	107.67	112.27
2	A	901	0UE	C22-C23-C24	-4.62	104.46	112.56
3	A	911	BNG	O1-C1-C2	4.57	115.44	108.30
3	A	906	BNG	O1-C1-C2	4.48	115.30	108.30
3	A	905	BNG	C1'-O1-C1	4.41	121.15	113.84
3	A	903	BNG	C1'-O1-C1	4.24	120.87	113.84
3	A	905	BNG	O1-C1-C2	4.02	114.58	108.30
3	A	907	BNG	C3-C4-C5	3.85	117.10	110.24
2	A	901	0UE	O31-N31-C31	-3.80	110.56	116.68
3	A	912	BNG	C3-C4-C5	3.59	116.65	110.24
3	A	905	BNG	O5-C5-C6	3.58	115.33	106.44
3	A	905	BNG	C1-C2-C3	3.52	117.32	110.00
3	A	904	BNG	C1-O5-C5	3.43	120.43	113.69
3	A	913	BNG	O3-C3-C2	3.40	118.22	110.35
2	A	901	0UE	C26-C25-N22	-3.40	102.50	112.21
2	A	901	0UE	C28-C27-C26	-3.38	97.27	114.42
3	A	906	BNG	C1'-O1-C1	3.36	119.42	113.84
3	A	907	BNG	O5-C5-C4	3.22	115.54	109.69
3	A	909	BNG	O1-C1-C2	3.12	113.17	108.30
3	A	908	BNG	O1-C1-C2	2.98	112.95	108.30
3	A	912	BNG	C1-O5-C5	2.97	119.52	113.69
3	A	907	BNG	C6-C5-C4	-2.84	106.34	113.00
3	A	914	BNG	O3-C3-C2	2.83	116.90	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	912	BNG	C4-C3-C2	2.82	115.75	110.82
3	A	905	BNG	O5-C5-C4	-2.72	104.76	109.69
2	A	901	0UE	C25-N22-C24	-2.69	117.85	122.84
3	A	906	BNG	O2-C2-C3	-2.68	104.15	110.35
2	A	901	0UE	C13-C14-N12	2.62	120.82	116.42
3	A	903	BNG	O5-C5-C6	2.57	112.82	106.44
3	A	911	BNG	O5-C1-C2	-2.54	104.97	110.35
2	A	901	0UE	C27-C28-C29	2.50	124.71	113.21
4	A	921	GOL	O2-C2-C3	-2.48	98.20	109.12
3	A	914	BNG	C4-C3-C2	-2.39	106.65	110.82
3	A	913	BNG	C4-C3-C2	-2.36	106.70	110.82
3	A	909	BNG	C1-O5-C5	2.32	118.23	113.69
3	A	914	BNG	O5-C5-C6	2.29	112.12	106.44
3	A	913	BNG	O6-C6-C5	-2.23	103.64	111.29
4	A	921	GOL	O1-C1-C2	2.23	120.89	110.20
3	A	912	BNG	O5-C5-C4	2.21	113.72	109.69
3	A	905	BNG	C4-C3-C2	2.16	114.60	110.82
3	A	906	BNG	C3-C4-C5	2.14	114.06	110.24
3	A	911	BNG	O1-C1'-C2'	2.10	116.94	109.56
3	A	907	BNG	O5-C5-C6	2.09	111.62	106.44
3	A	908	BNG	C4-C3-C2	-2.06	107.23	110.82
3	A	909	BNG	O5-C5-C4	2.06	113.43	109.69
2	A	901	0UE	O13-C14-N12	-2.04	119.17	123.01

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	901	0UE	N31

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	0UE	O12-C11-C12-C13
2	A	901	0UE	N11-C11-C12-C13
2	A	901	0UE	C17-C18-C19-N21
2	A	901	0UE	C18-C19-N21-C21
2	A	901	0UE	N11-C39-C40-C41
3	A	904	BNG	O5-C1-O1-C1'
3	A	905	BNG	C2-C1-O1-C1'
3	A	906	BNG	O5-C1-O1-C1'
4	A	917	GOL	O1-C1-C2-O2
4	A	917	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	918	GOL	C1-C2-C3-O3
4	A	920	GOL	O1-C1-C2-C3
4	A	920	GOL	C1-C2-C3-O3
4	A	920	GOL	O2-C2-C3-O3
3	A	906	BNG	O5-C5-C6-O6
3	A	904	BNG	O5-C5-C6-O6
3	A	908	BNG	O5-C5-C6-O6
3	A	905	BNG	O5-C5-C6-O6
3	A	909	BNG	O5-C1-O1-C1'
2	A	901	0UE	N12-C15-C16-C17
3	A	905	BNG	C4-C5-C6-O6
3	A	904	BNG	C4-C5-C6-O6
3	A	903	BNG	C2-C1-O1-C1'
3	A	908	BNG	C4-C5-C6-O6
2	A	901	0UE	C11-C12-C13-C14
3	A	909	BNG	O5-C5-C6-O6
2	A	901	0UE	N22-C25-C26-C27
3	A	906	BNG	C3'-C4'-C5'-C6'
3	A	907	BNG	O1-C1'-C2'-C3'
3	A	906	BNG	C4-C5-C6-O6
2	A	901	0UE	C12-C13-C14-N12
2	A	901	0UE	C12-C13-C14-O13
3	A	912	BNG	C2-C1-O1-C1'
3	A	909	BNG	O1-C1'-C2'-C3'
3	A	913	BNG	C3'-C4'-C5'-C6'
3	A	912	BNG	C4'-C5'-C6'-C7'
3	A	914	BNG	C4'-C5'-C6'-C7'
3	A	907	BNG	C3'-C4'-C5'-C6'
3	A	905	BNG	O5-C1-O1-C1'
3	A	903	BNG	C4'-C5'-C6'-C7'
3	A	909	BNG	C5'-C6'-C7'-C8'
3	A	913	BNG	C2'-C3'-C4'-C5'
3	A	912	BNG	O1-C1'-C2'-C3'
4	A	918	GOL	O2-C2-C3-O3
4	A	920	GOL	O1-C1-C2-O2
2	A	901	0UE	C26-C27-C28-C29
3	A	908	BNG	C2'-C3'-C4'-C5'
3	A	905	BNG	C3'-C4'-C5'-C6'
3	A	905	BNG	O1-C1'-C2'-C3'
3	A	904	BNG	C1'-C2'-C3'-C4'
3	A	908	BNG	O1-C1'-C2'-C3'
3	A	910	BNG	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
3	A	903	BNG	O1-C1'-C2'-C3'
3	A	912	BNG	O5-C1-O1-C1'
3	A	906	BNG	C1'-C2'-C3'-C4'
3	A	902	BNG	C5'-C6'-C7'-C8'
3	A	908	BNG	C1'-C2'-C3'-C4'
3	A	909	BNG	C3'-C4'-C5'-C6'
3	A	914	BNG	C2'-C3'-C4'-C5'
3	A	906	BNG	C5'-C6'-C7'-C8'
3	A	912	BNG	O5-C5-C6-O6
2	A	901	0UE	C16-C17-C18-C19
3	A	902	BNG	C2'-C3'-C4'-C5'
3	A	908	BNG	C3'-C4'-C5'-C6'
3	A	906	BNG	C2-C1-O1-C1'
3	A	910	BNG	C6'-C7'-C8'-C9'
3	A	908	BNG	C4'-C5'-C6'-C7'
3	A	904	BNG	C2'-C1'-O1-C1
3	A	907	BNG	C2'-C1'-O1-C1
3	A	912	BNG	C2'-C1'-O1-C1
3	A	910	BNG	C2'-C3'-C4'-C5'
3	A	911	BNG	C3'-C4'-C5'-C6'
3	A	913	BNG	O1-C1'-C2'-C3'
3	A	906	BNG	C6'-C7'-C8'-C9'
3	A	905	BNG	C2'-C3'-C4'-C5'
3	A	904	BNG	C6'-C7'-C8'-C9'
3	A	911	BNG	C5'-C6'-C7'-C8'
4	A	916	GOL	O1-C1-C2-O2
3	A	903	BNG	O5-C1-O1-C1'
3	A	909	BNG	C4-C5-C6-O6
3	A	904	BNG	C4'-C5'-C6'-C7'
4	A	916	GOL	C1-C2-C3-O3
3	A	914	BNG	C3'-C4'-C5'-C6'
3	A	902	BNG	C2'-C1'-O1-C1
3	A	904	BNG	C5'-C6'-C7'-C8'
3	A	914	BNG	O1-C1'-C2'-C3'
3	A	906	BNG	C2'-C3'-C4'-C5'
3	A	903	BNG	C2'-C3'-C4'-C5'
4	A	916	GOL	O1-C1-C2-C3
3	A	912	BNG	C6'-C7'-C8'-C9'
3	A	908	BNG	C6'-C7'-C8'-C9'
3	A	906	BNG	C4'-C5'-C6'-C7'
3	A	912	BNG	C3'-C4'-C5'-C6'
3	A	914	BNG	C5'-C6'-C7'-C8'

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Mol	Chain	Res	Type	Atoms
3	A	913	BNG	C6'-C7'-C8'-C9'
3	A	906	BNG	C2'-C1'-O1-C1
3	A	908	BNG	O5-C1-O1-C1'
3	A	912	BNG	C5'-C6'-C7'-C8'

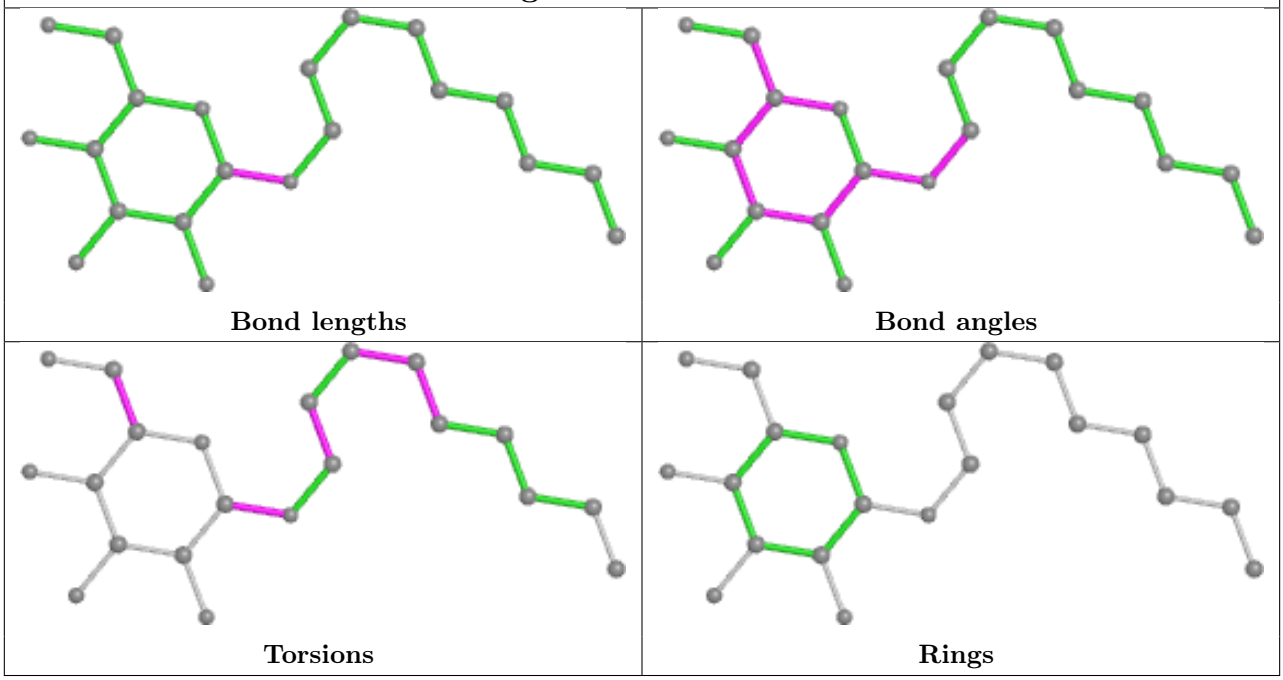
There are no ring outliers.

7 monomers are involved in 18 short contacts:

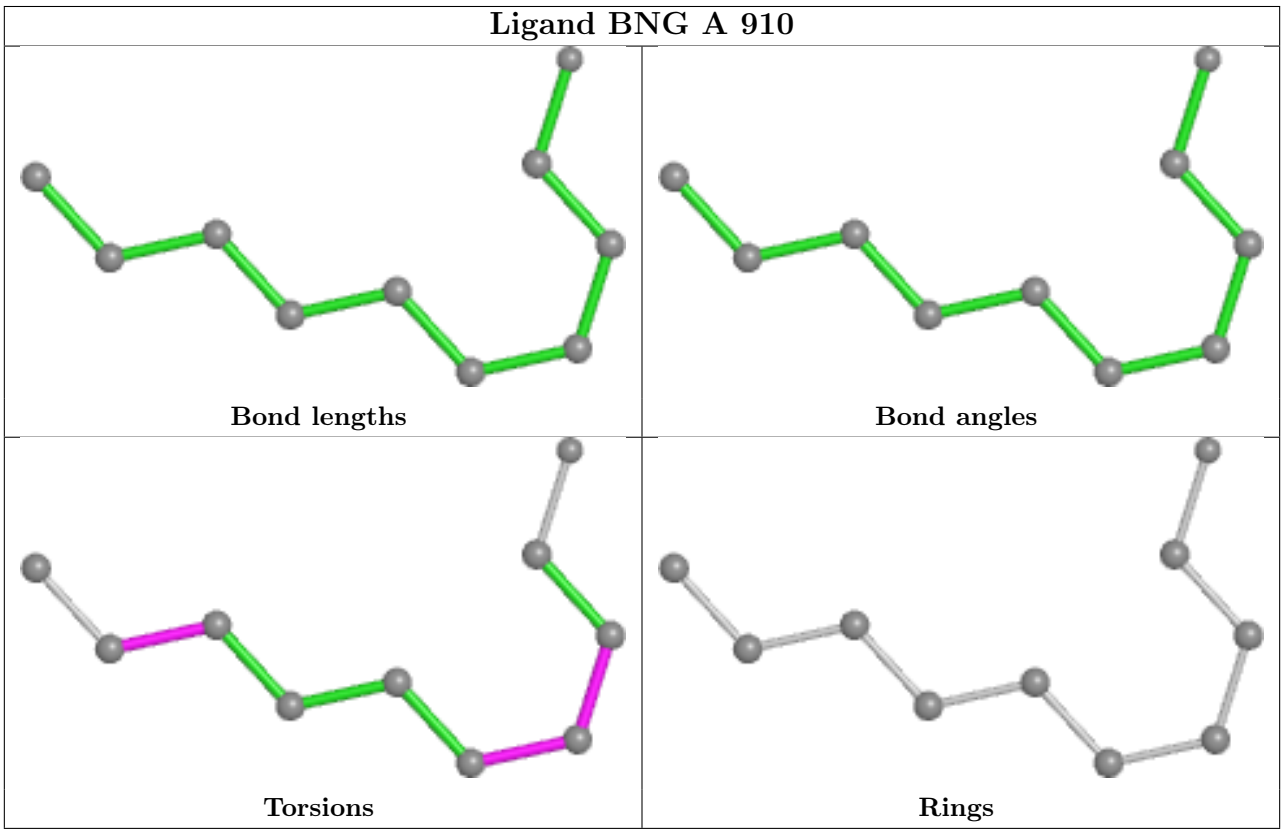
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	905	BNG	1	0
3	A	904	BNG	1	0
3	A	911	BNG	1	0
3	A	906	BNG	2	0
2	A	901	0UE	10	0
4	A	920	GOL	1	0
3	A	913	BNG	2	0

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 then 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.

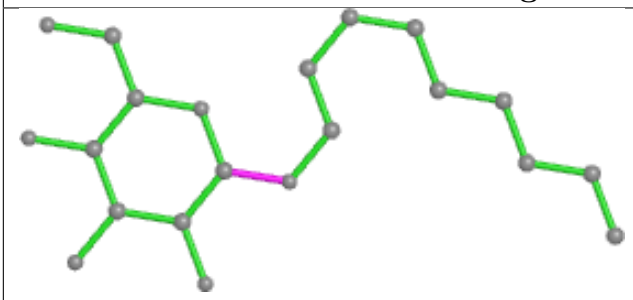
Ligand BNG A 905



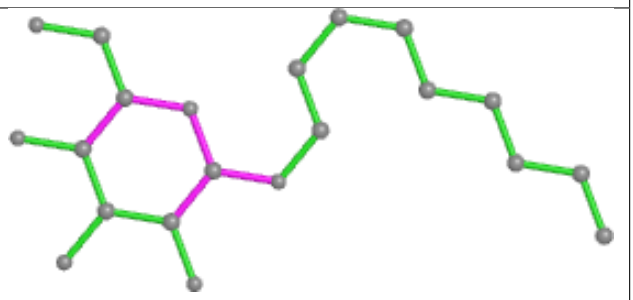
Ligand BNG A 910



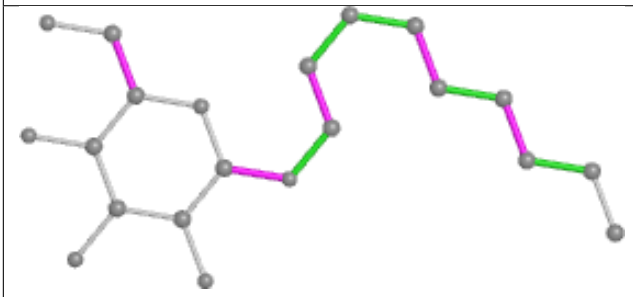
Ligand BNG A 909



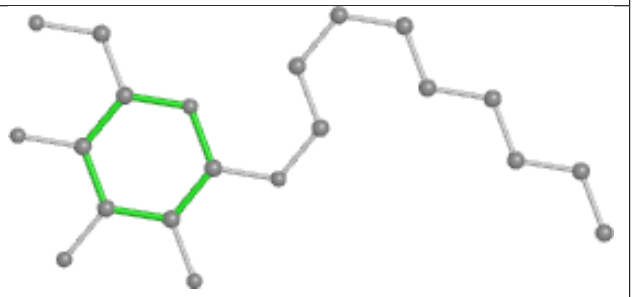
Bond lengths



Bond angles

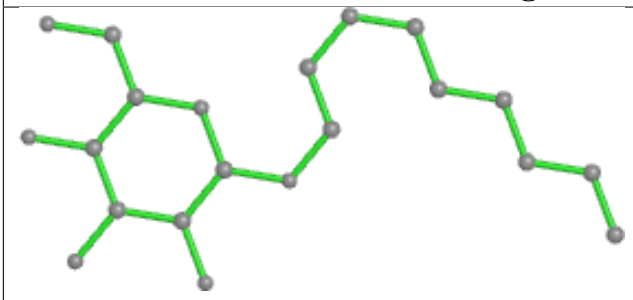


Torsions

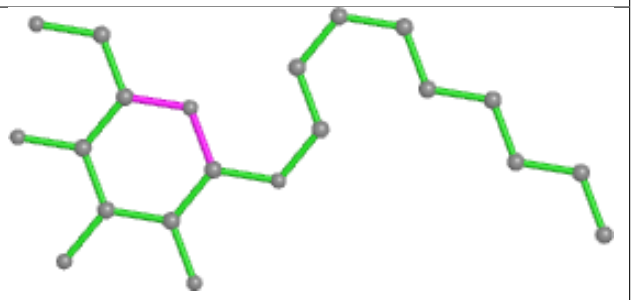


Rings

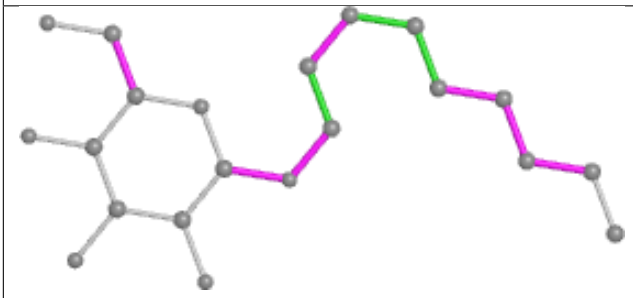
Ligand BNG A 904



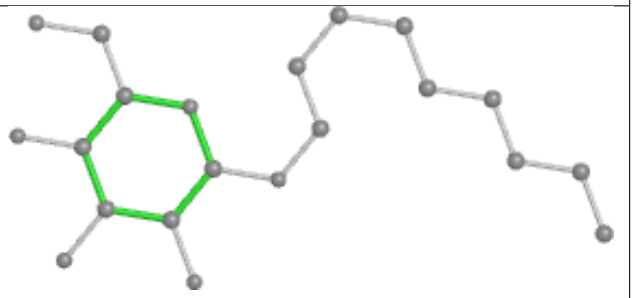
Bond lengths



Bond angles

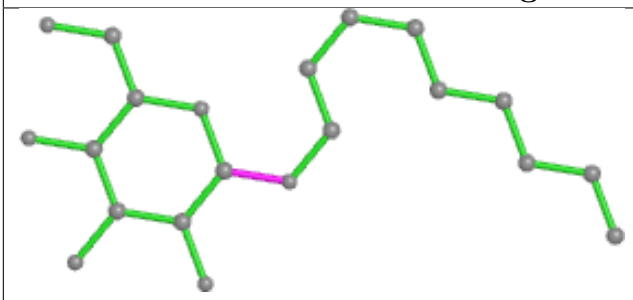


Torsions

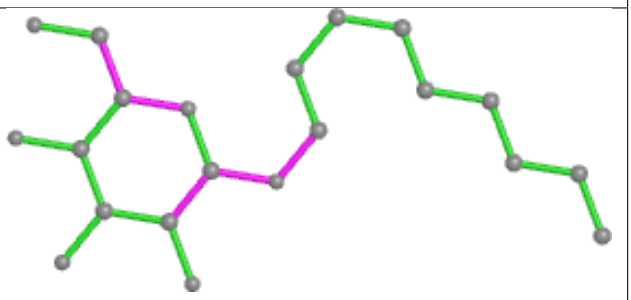


Rings

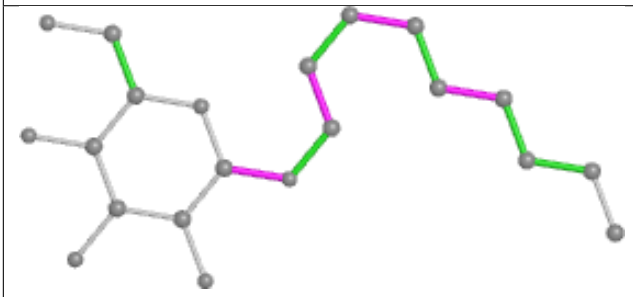
Ligand BNG A 903



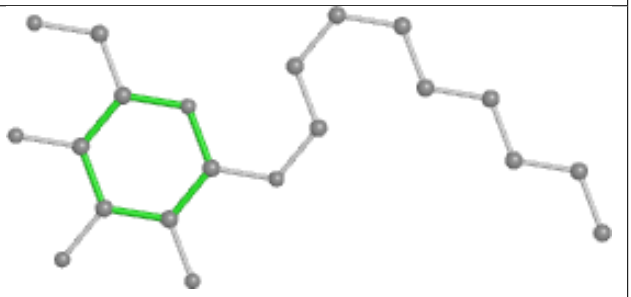
Bond lengths



Bond angles

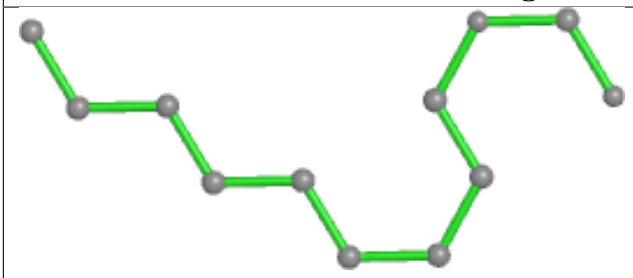


Torsions

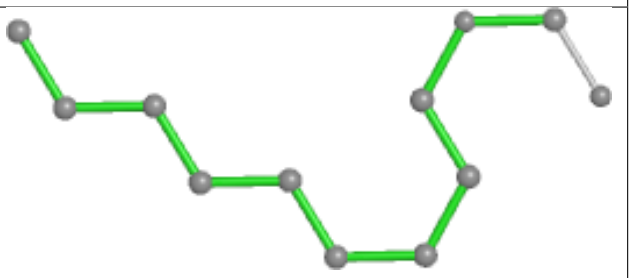


Rings

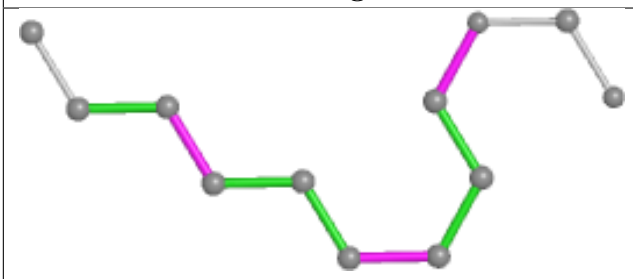
Ligand BNG A 902



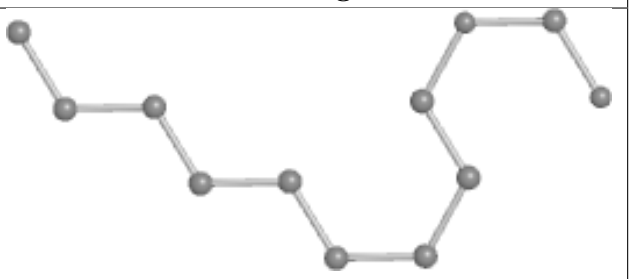
Bond lengths



Bond angles

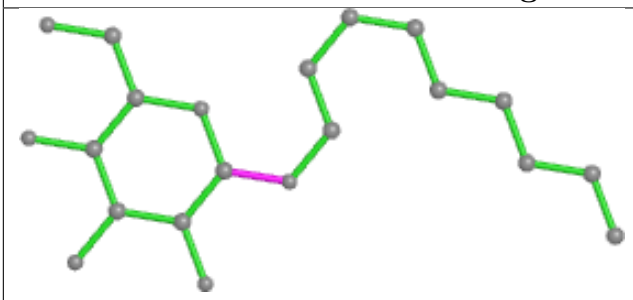


Torsions



Rings

Ligand BNG A 911



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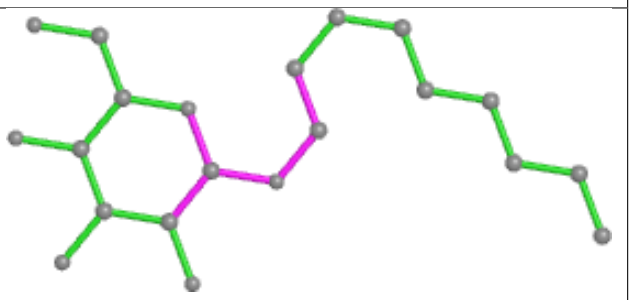
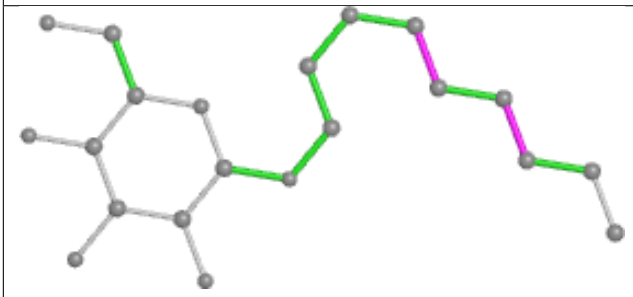


Bond angles



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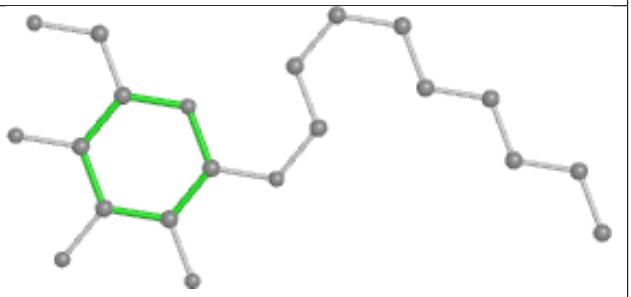
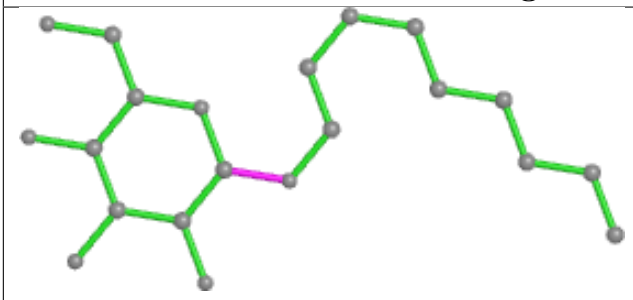


Rings

Ligand BNG A 907



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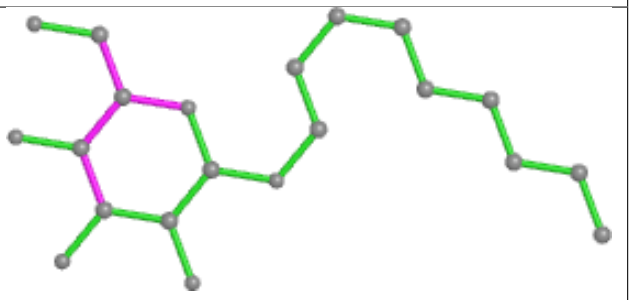

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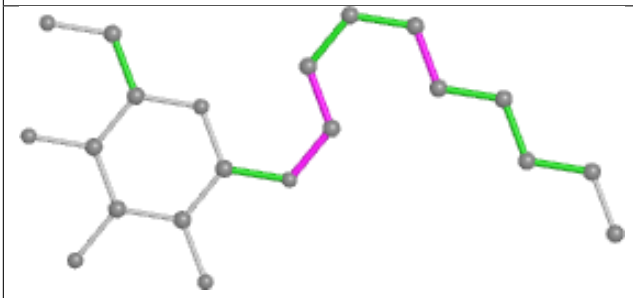

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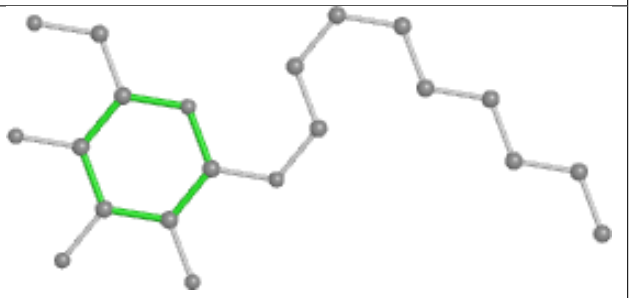
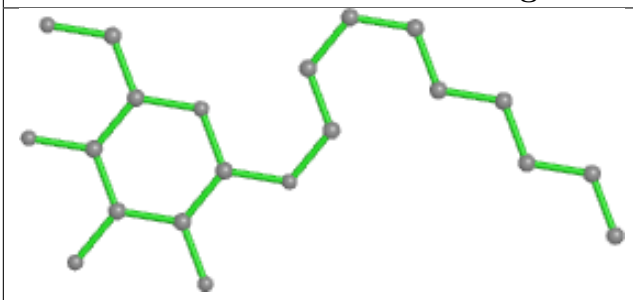


Rings

Ligand BNG A 908



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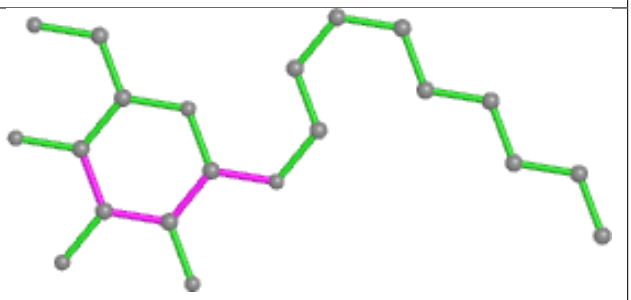
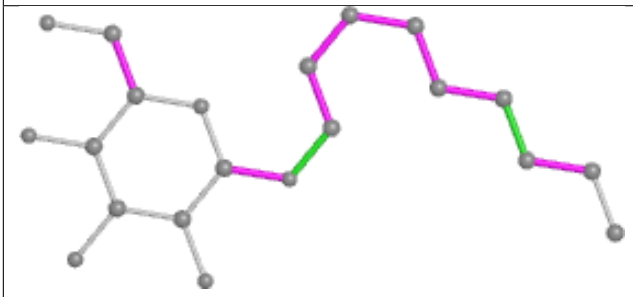


Bond angles



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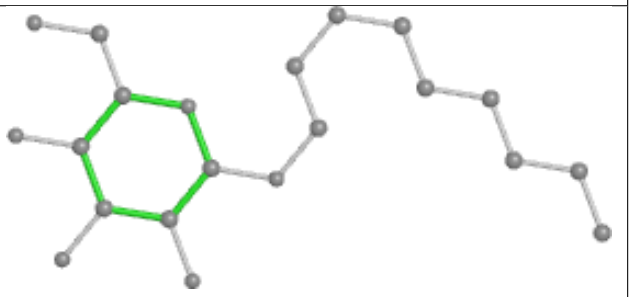
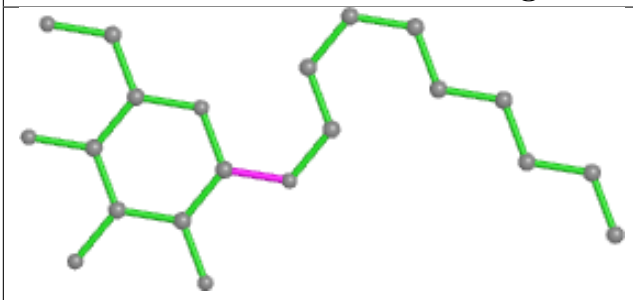
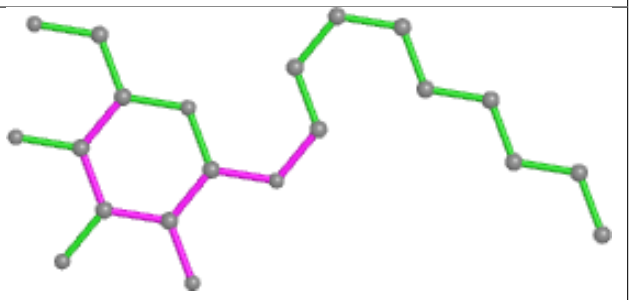


Rings

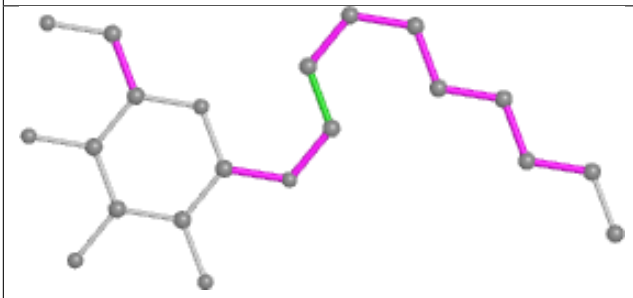
Ligand BNG A 906



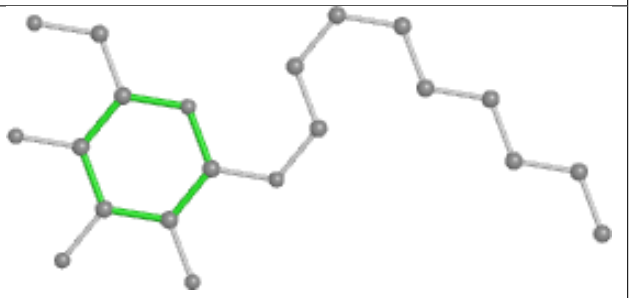
Bond lengths



Bond angles

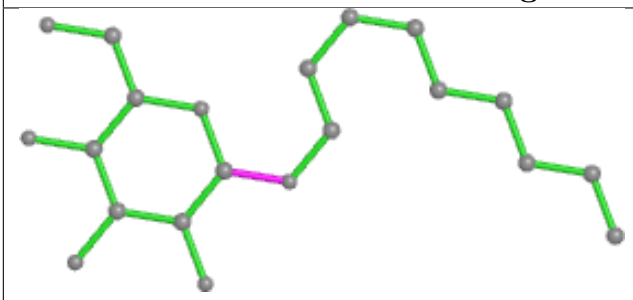


Torsions



Rings

Ligand BNG A 912



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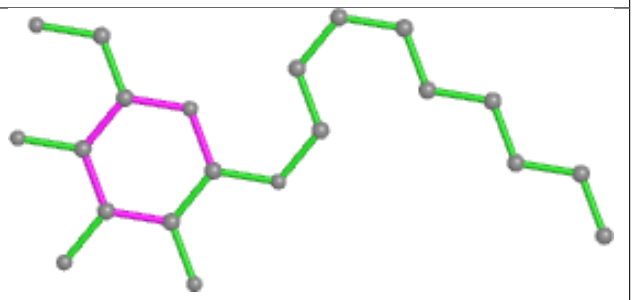
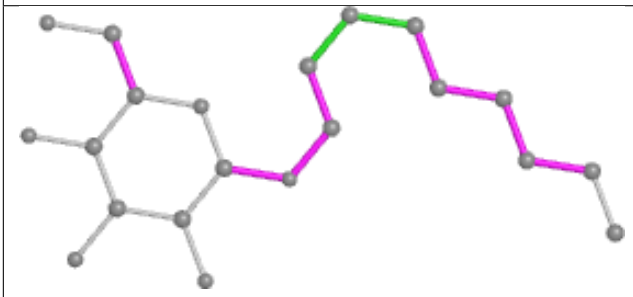


Bond angles



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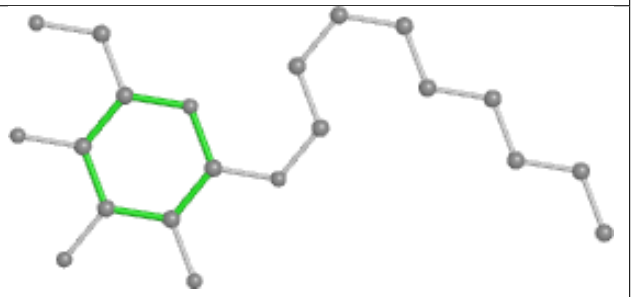
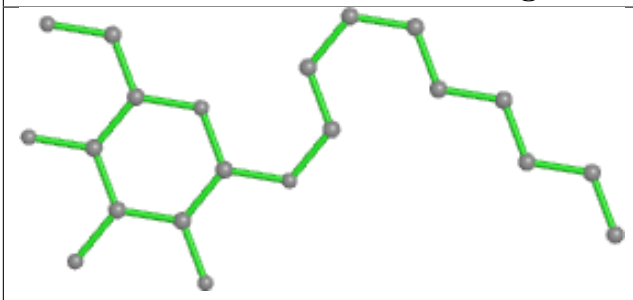
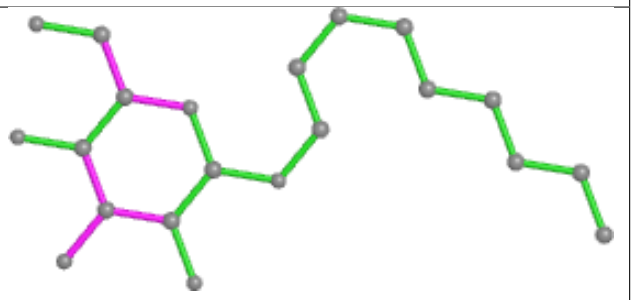


Rings

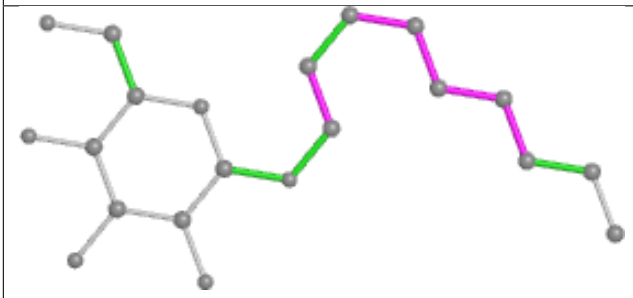
Ligand BNG A 914



Bond lengths



Bond angles



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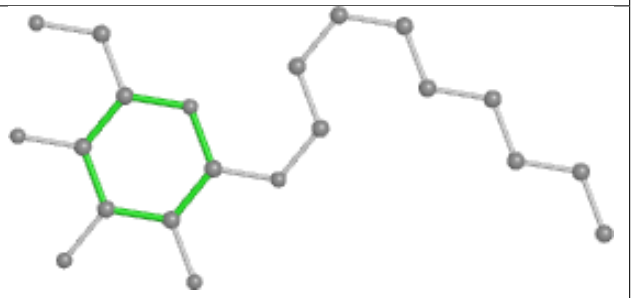
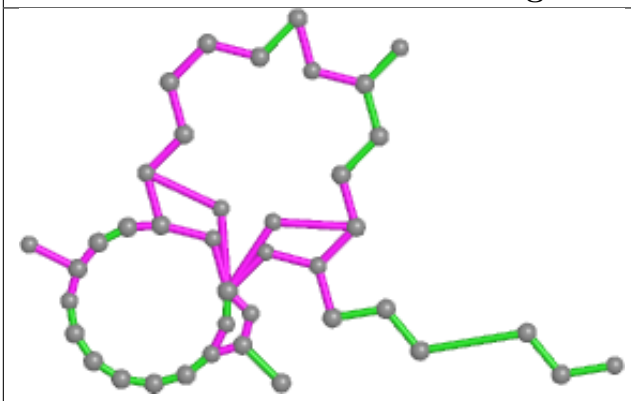
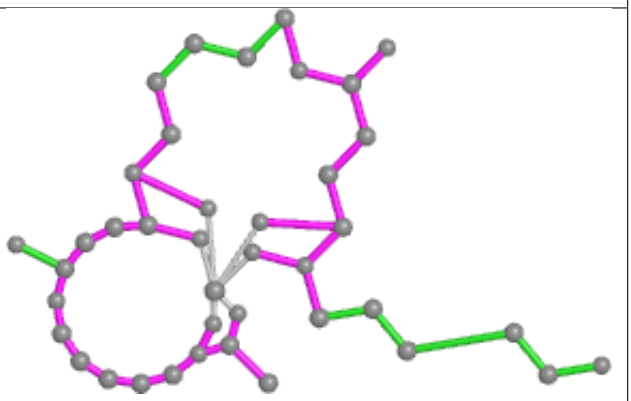


Rings

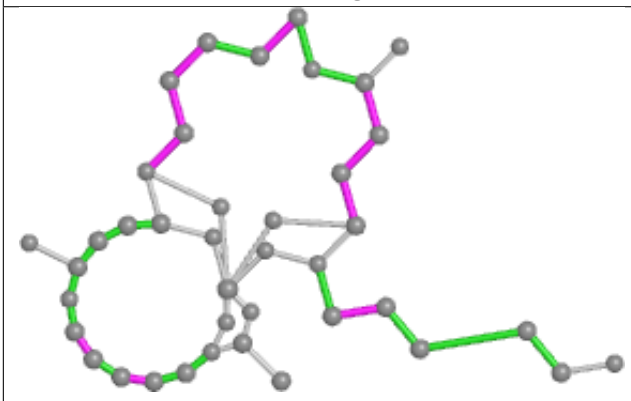
Ligand 0UE A 901



Bond lengths



Bond angles



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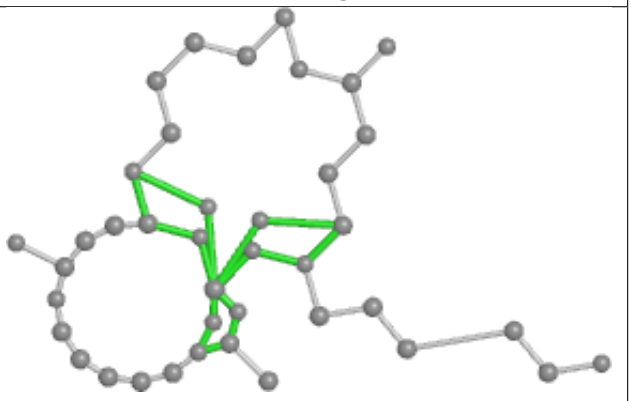
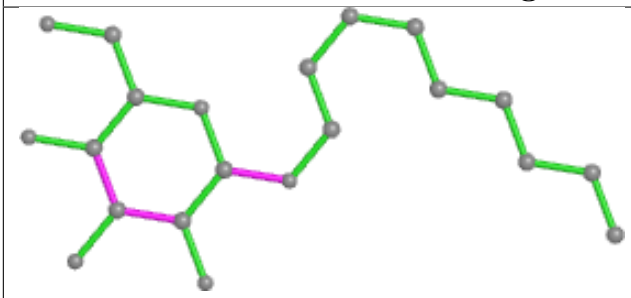
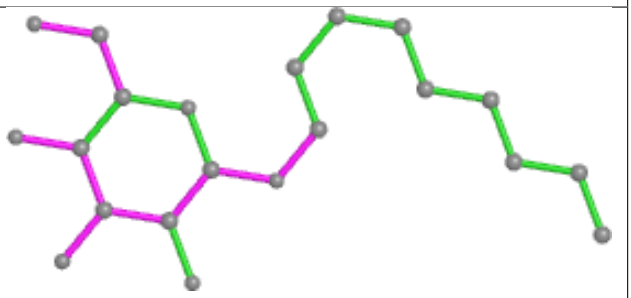


Rings

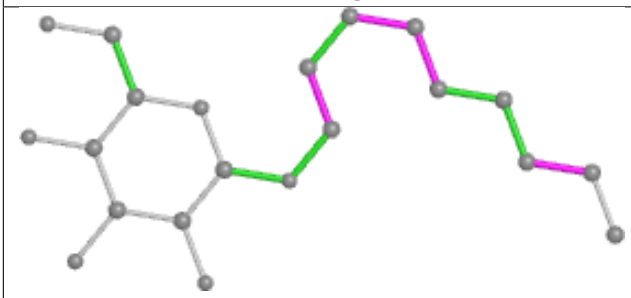
Ligand BNG A 913



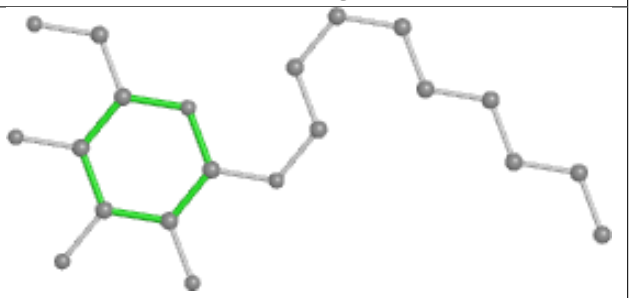
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	677/677 (100%)	-0.17	6 (0%)	84	84	29, 45, 78, 112	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	614	ALA	4.3
1	A	663	PHE	3.5
1	A	684	SER	3.5
1	A	144	VAL	2.3
1	A	617	THR	2.2
1	A	615	SER	2.1

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 monosaccharides 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, 95^{th} 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
3	BNG	A	912	21/21	0.42	0.26	67,107,133,135	0

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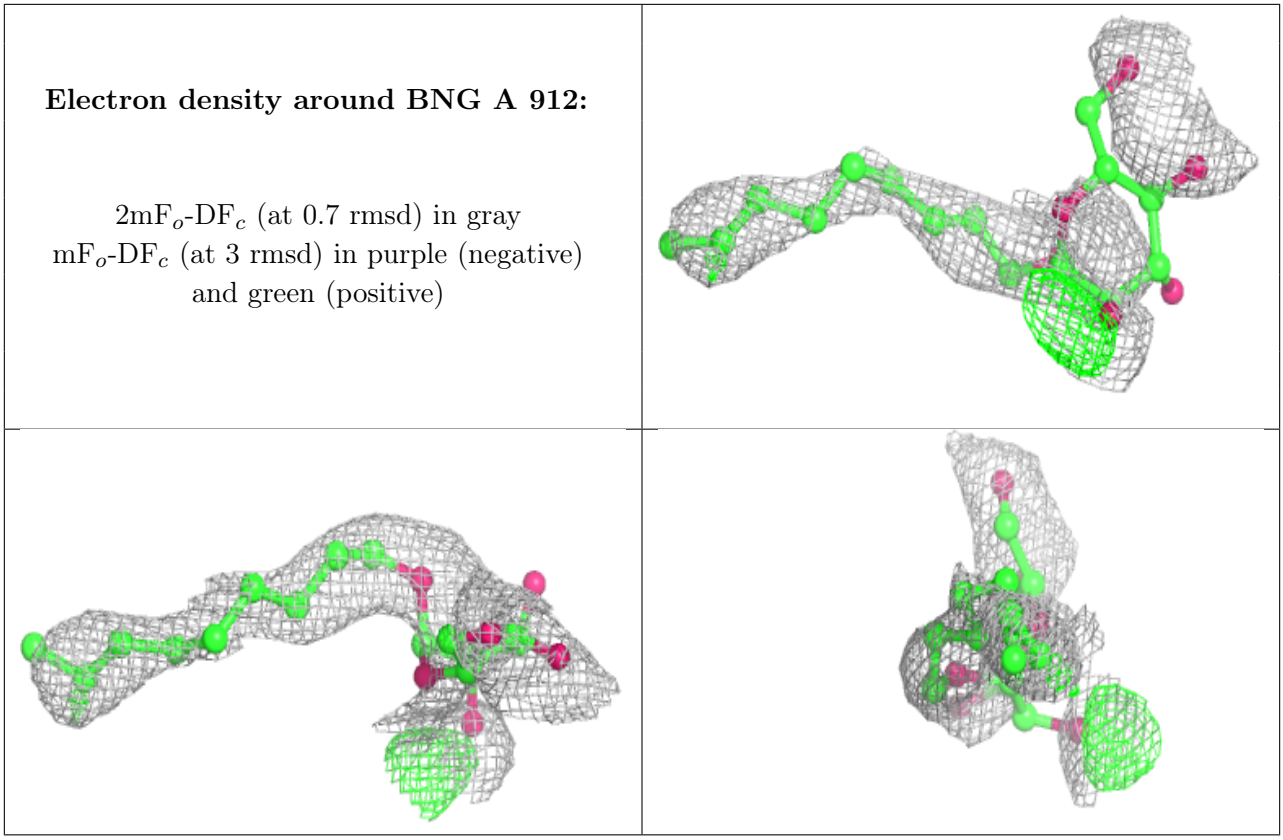
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BNG	A	905	21/21	0.51	0.29	61,102,119,131	0
3	BNG	A	909	21/21	0.55	0.26	64,89,115,118	0
3	BNG	A	902	12/21	0.56	0.33	70,81,105,106	0
3	BNG	A	911	21/21	0.57	0.24	55,77,96,103	0
3	BNG	A	904	21/21	0.61	0.31	53,76,98,104	0
3	BNG	A	908	21/21	0.64	0.23	61,87,98,102	0
4	GOL	A	917	6/6	0.66	0.30	77,87,98,102	0
3	BNG	A	903	21/21	0.67	0.20	64,80,100,111	0
4	GOL	A	920	6/6	0.67	0.14	57,61,66,70	0
3	BNG	A	906	21/21	0.68	0.28	61,78,121,127	0
4	GOL	A	922	6/6	0.69	0.20	72,84,86,89	0
3	BNG	A	913	21/21	0.73	0.21	51,77,88,99	0
3	BNG	A	907	21/21	0.76	0.23	60,109,127,129	0
3	BNG	A	910	10/21	0.77	0.15	72,78,90,93	0
5	SO4	A	925	5/5	0.79	0.37	104,105,118,118	0
3	BNG	A	914	21/21	0.81	0.23	65,83,99,102	0
5	SO4	A	923	5/5	0.82	0.22	77,95,110,113	0
4	GOL	A	916	6/6	0.83	0.23	54,64,73,99	0
6	NA	A	928	1/1	0.84	0.21	76,76,76,76	0
5	SO4	A	926	5/5	0.87	0.24	99,113,117,120	0
4	GOL	A	921	6/6	0.90	0.17	47,56,66,68	0
4	GOL	A	919	6/6	0.93	0.10	45,79,89,92	0
4	GOL	A	918	6/6	0.94	0.09	43,49,51,54	0
2	0UE	A	901	40/40	0.95	0.13	37,47,66,68	0
4	GOL	A	915	6/6	0.97	0.09	31,34,36,38	0
6	NA	A	927	1/1	0.98	0.12	42,42,42,42	0
5	SO4	A	924	5/5	0.99	0.07	42,46,56,59	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.

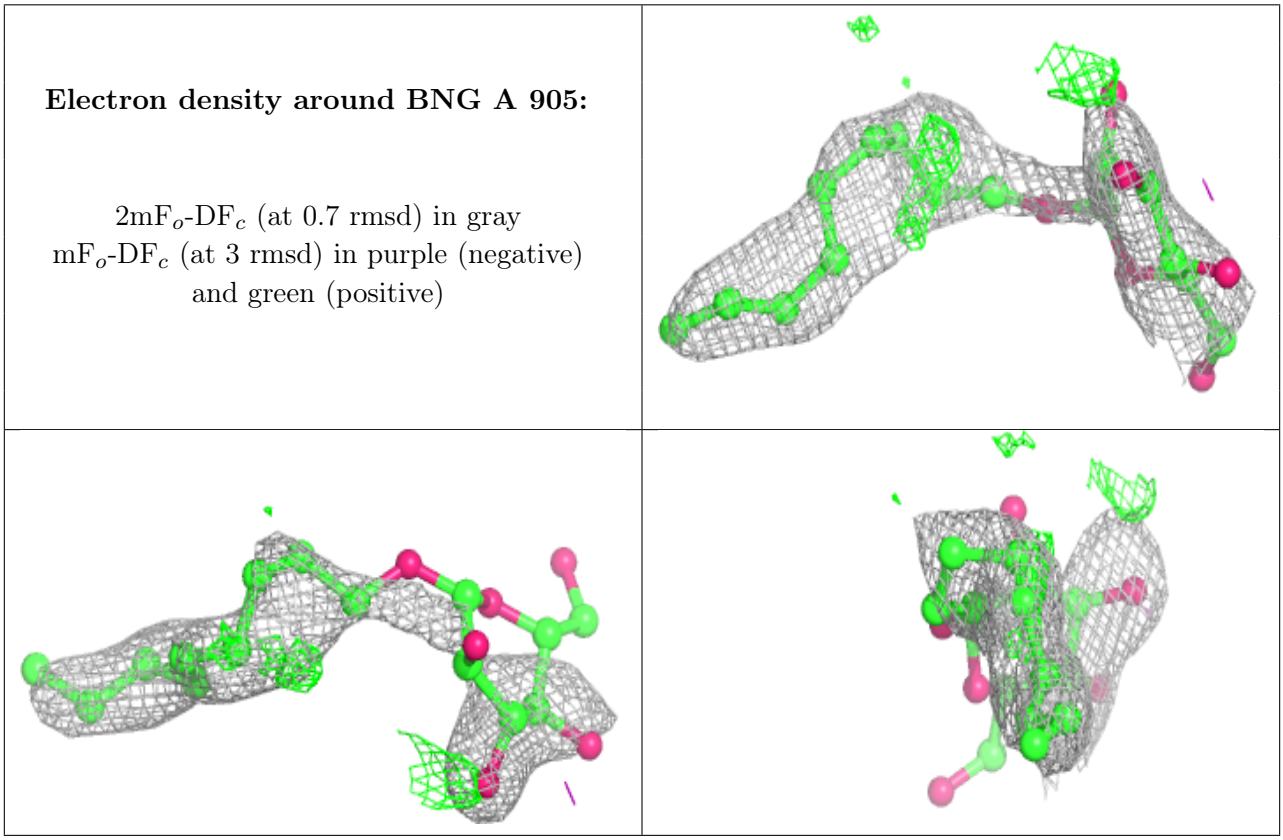
Electron density around BNG A 912:

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



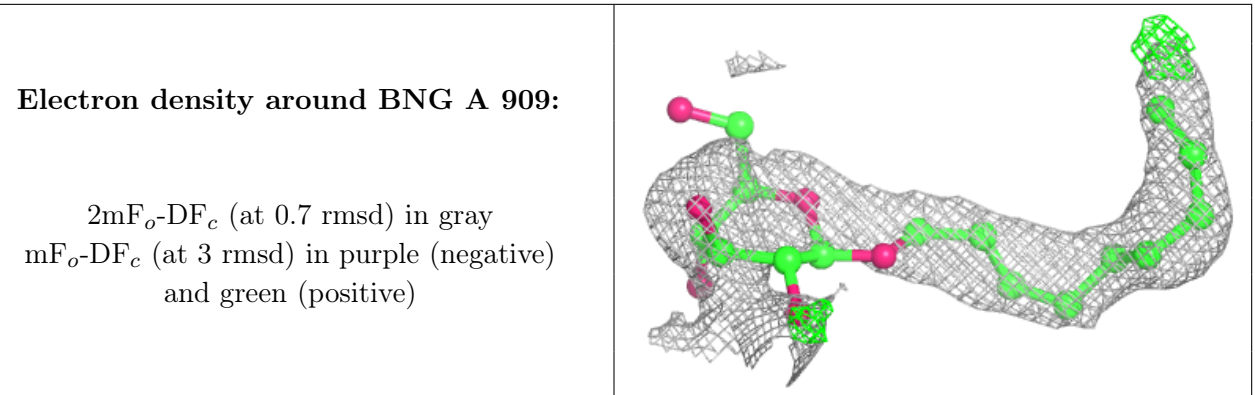
Electron density around BNG A 905:

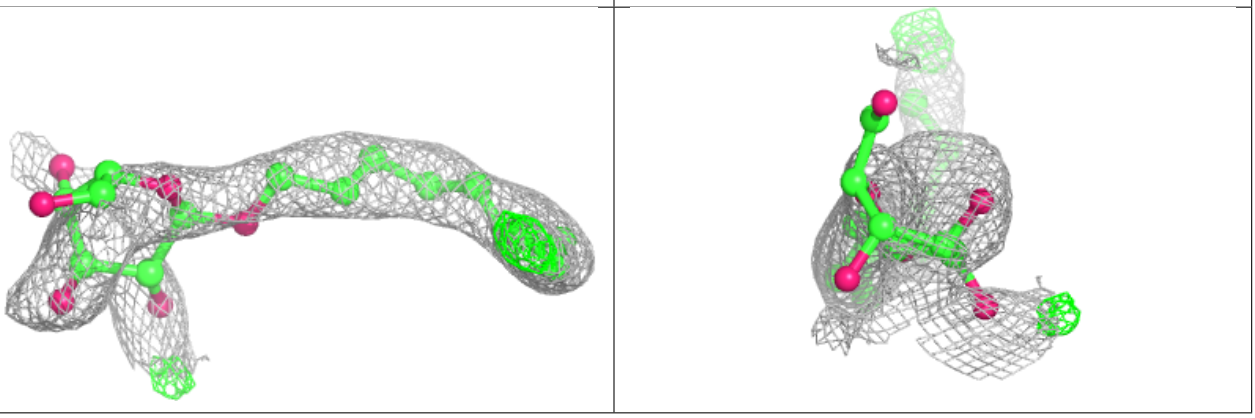
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BNG A 909:

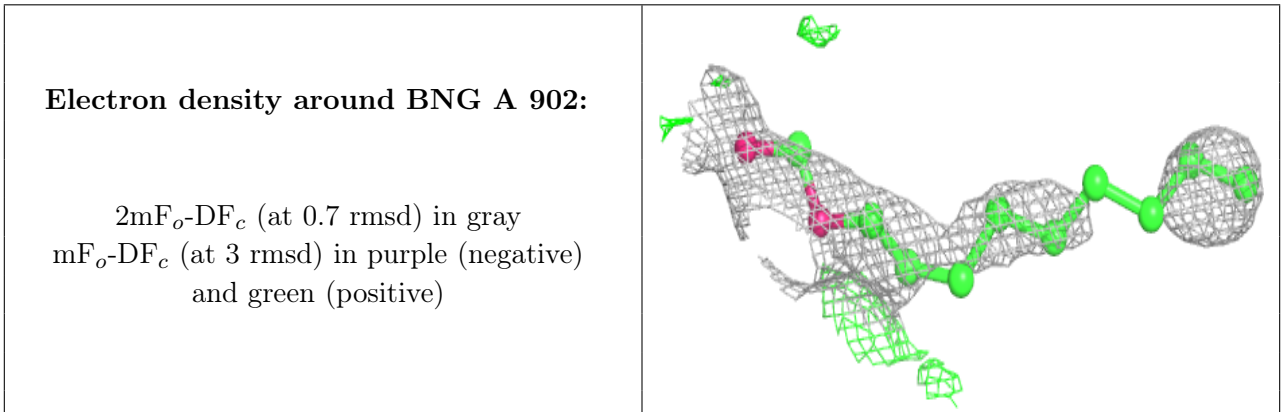
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

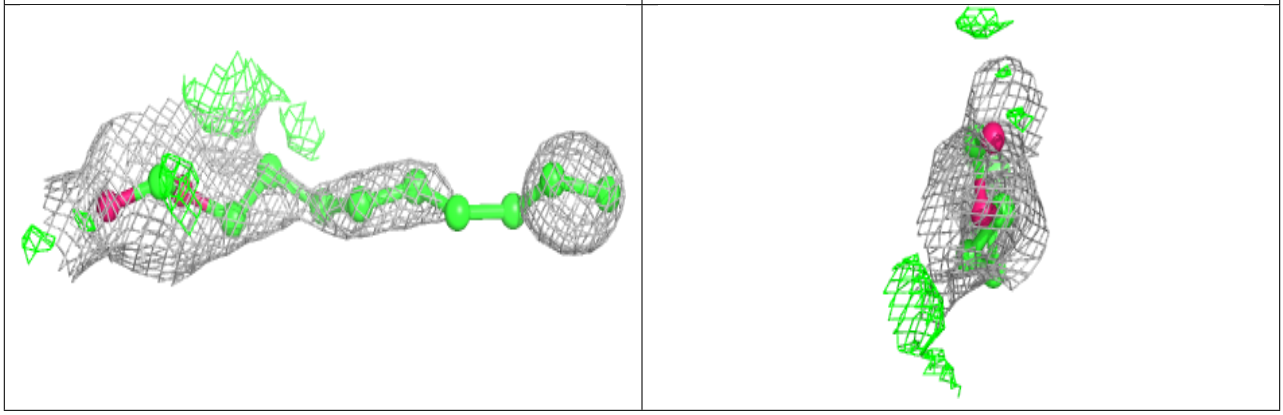




Electron density around BNG A 902:

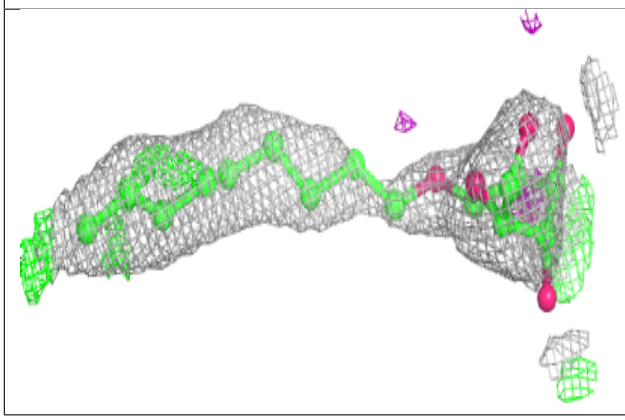
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

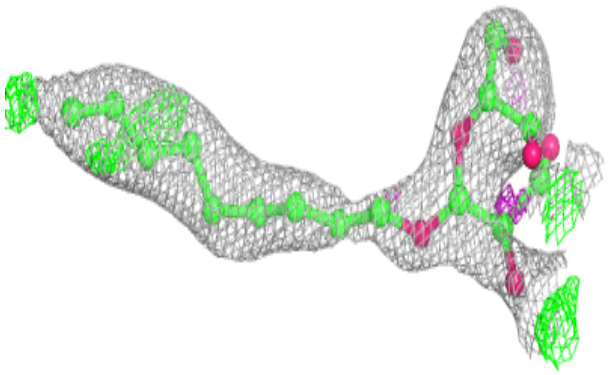


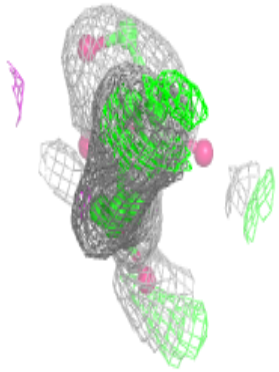


Electron density around BNG A 911:

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

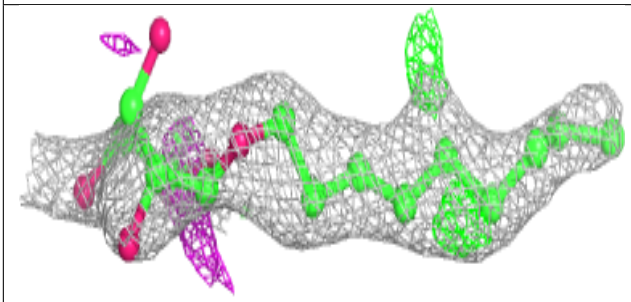


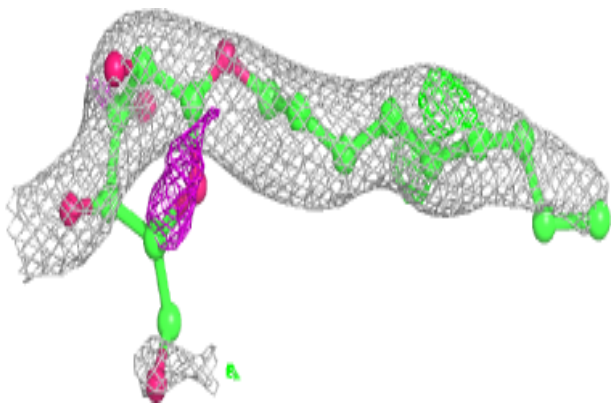


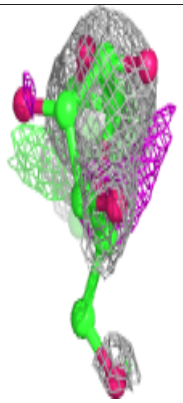


Electron density around BNG A 904:

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

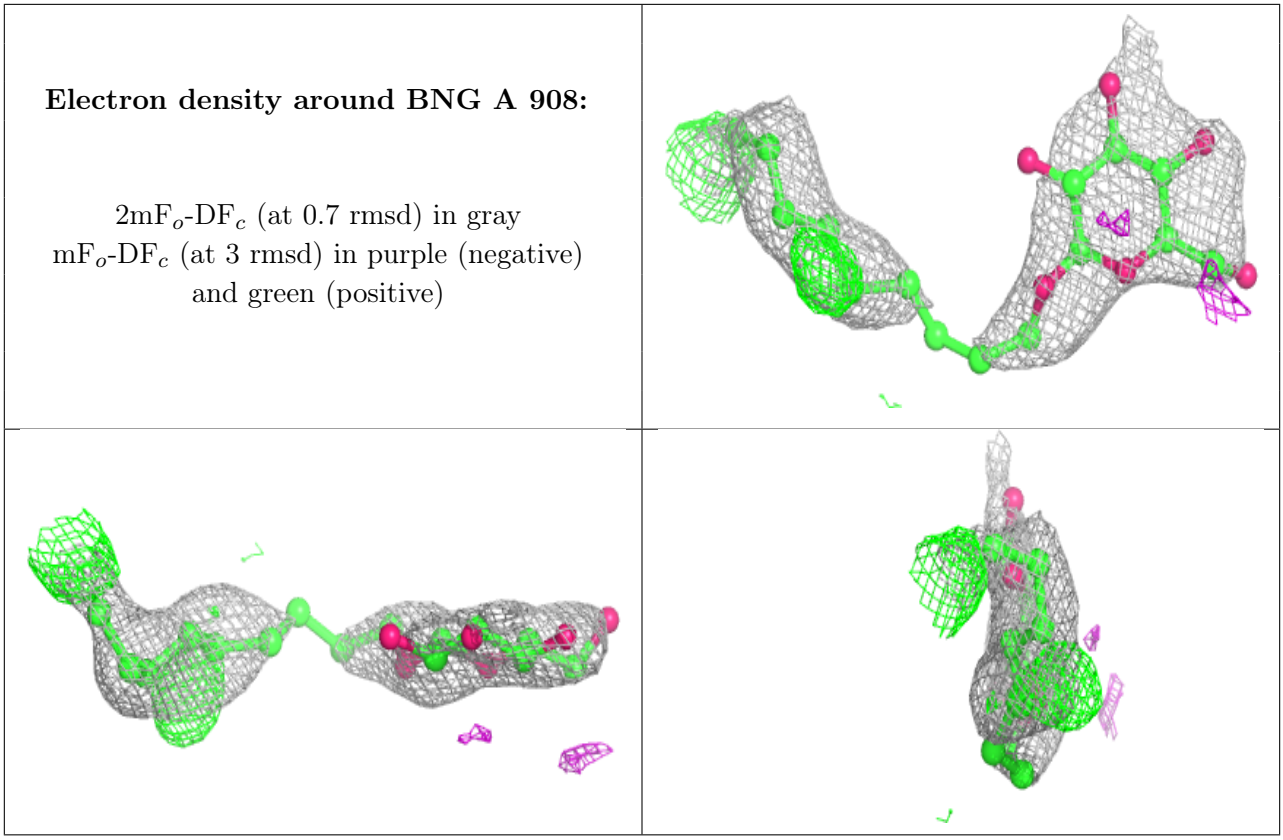






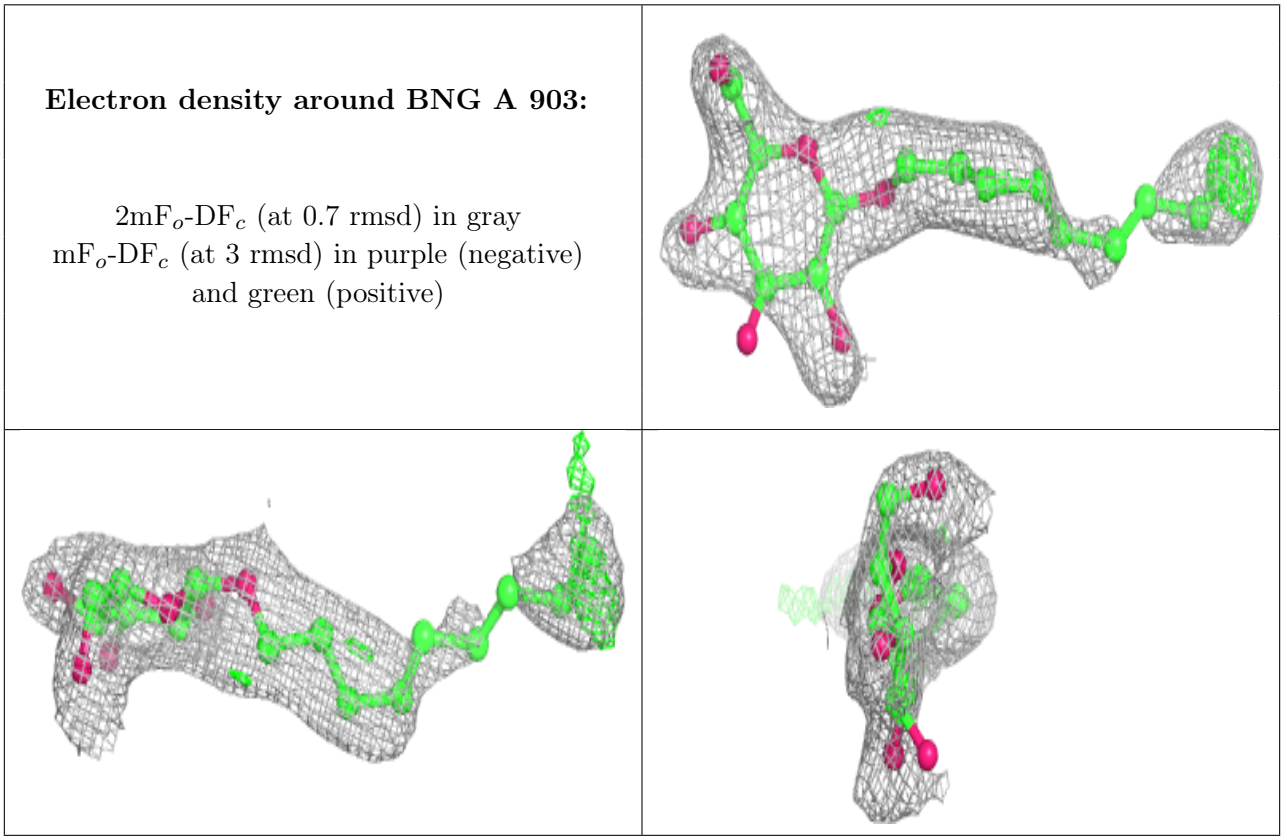
Electron density around BNG A 908:

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



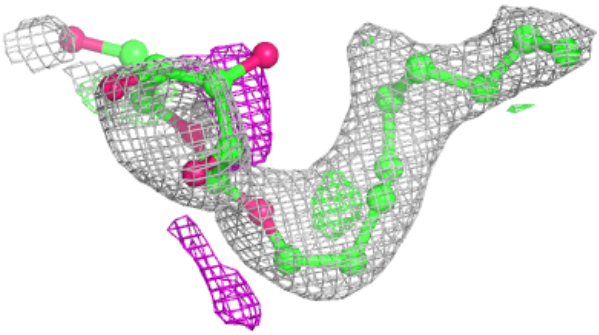
Electron density around BNG A 903:

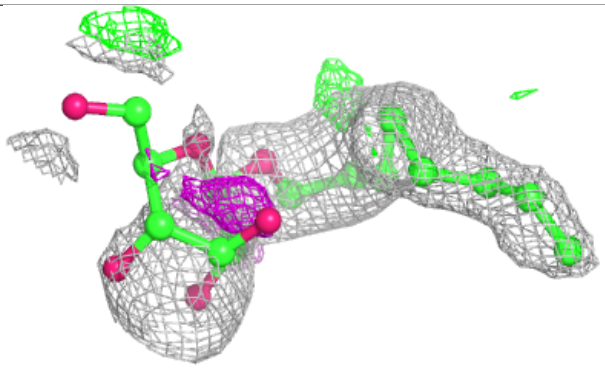
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

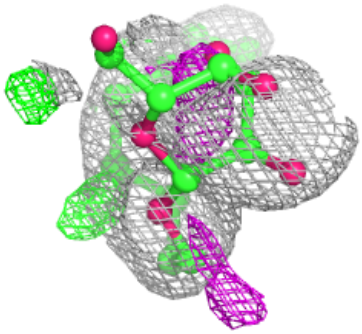


Electron density around BNG A 906:

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

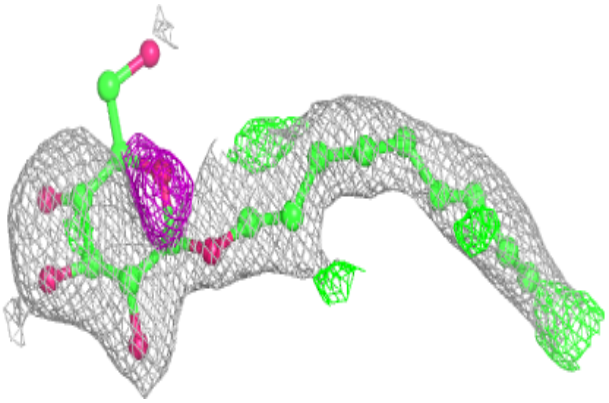


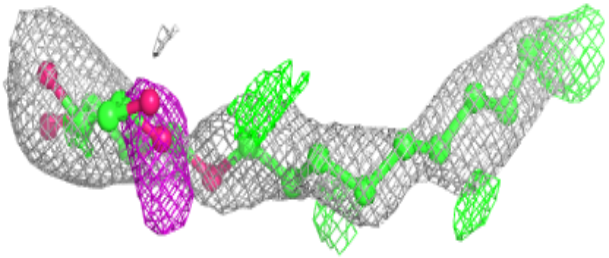


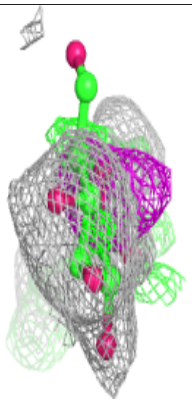


Electron density around BNG A 913:

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

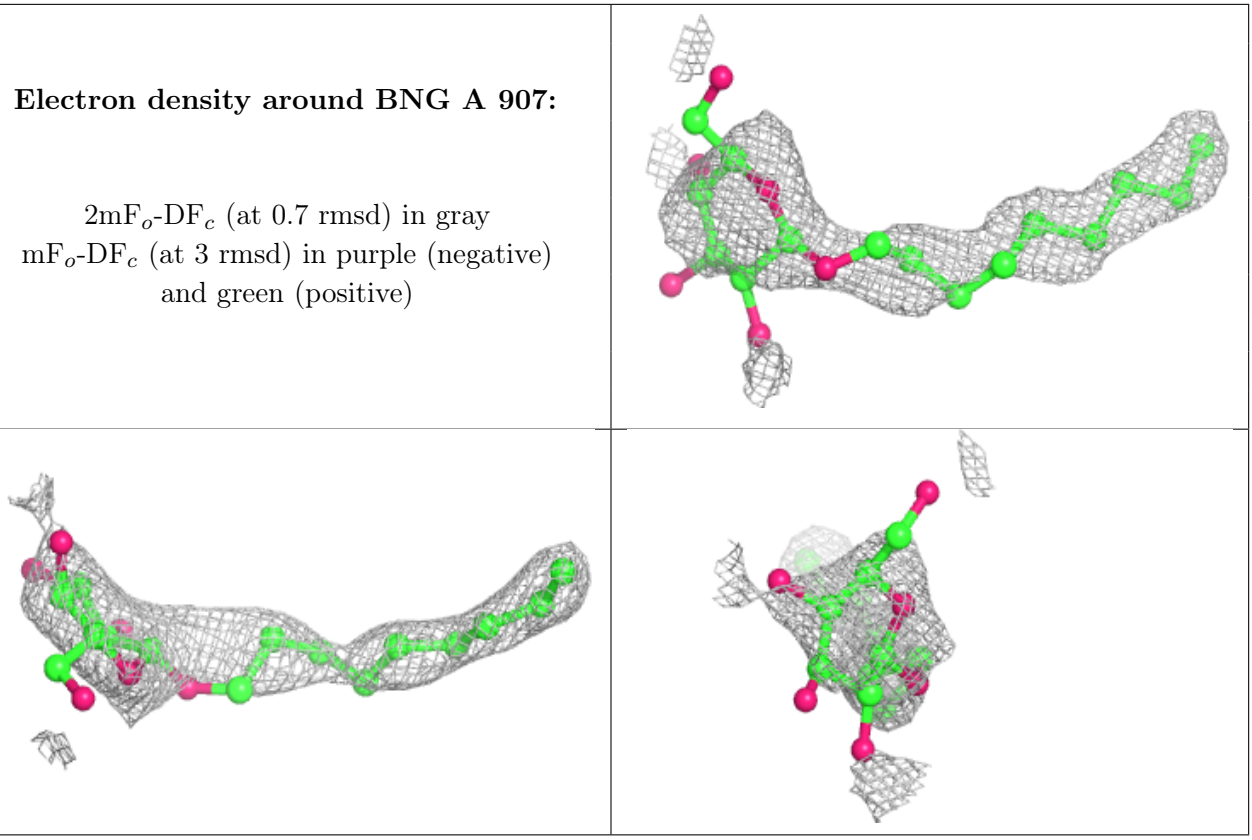






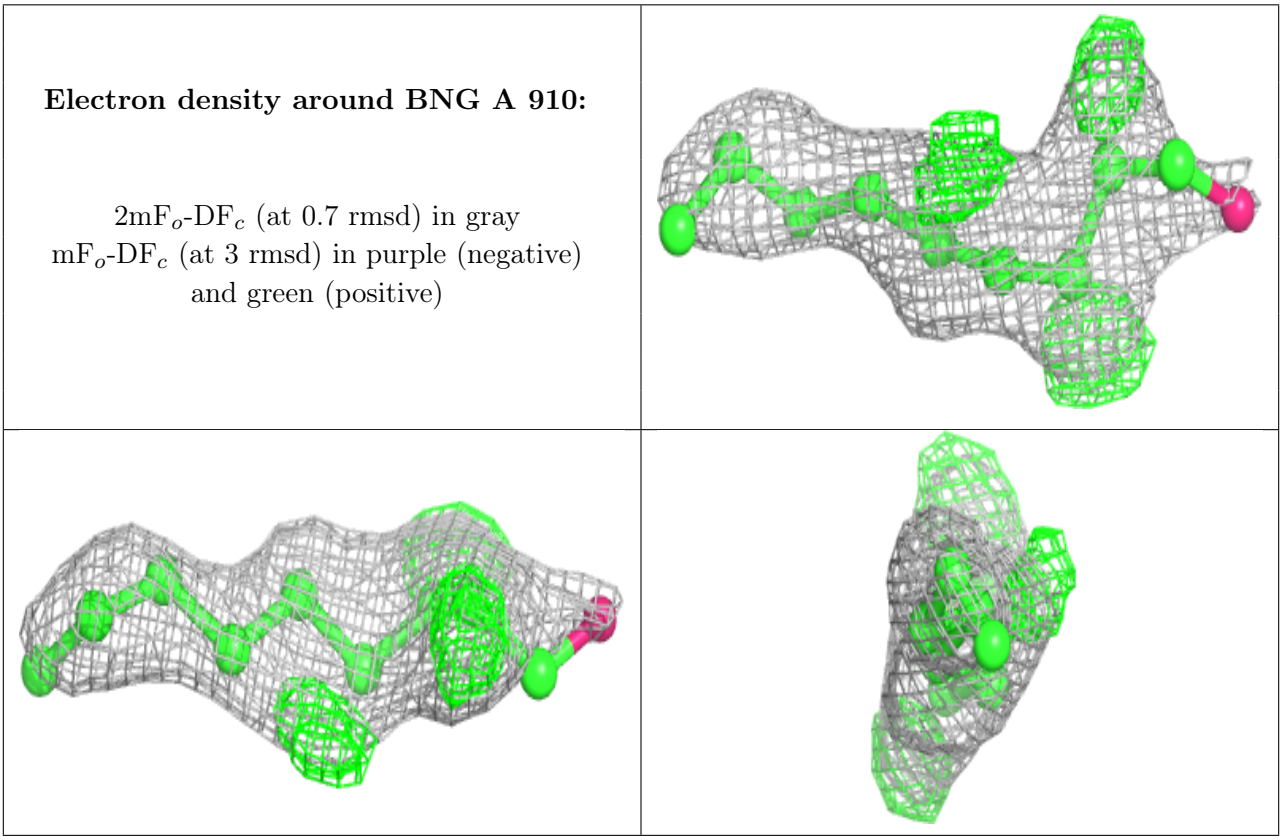
Electron density around BNG A 907:

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



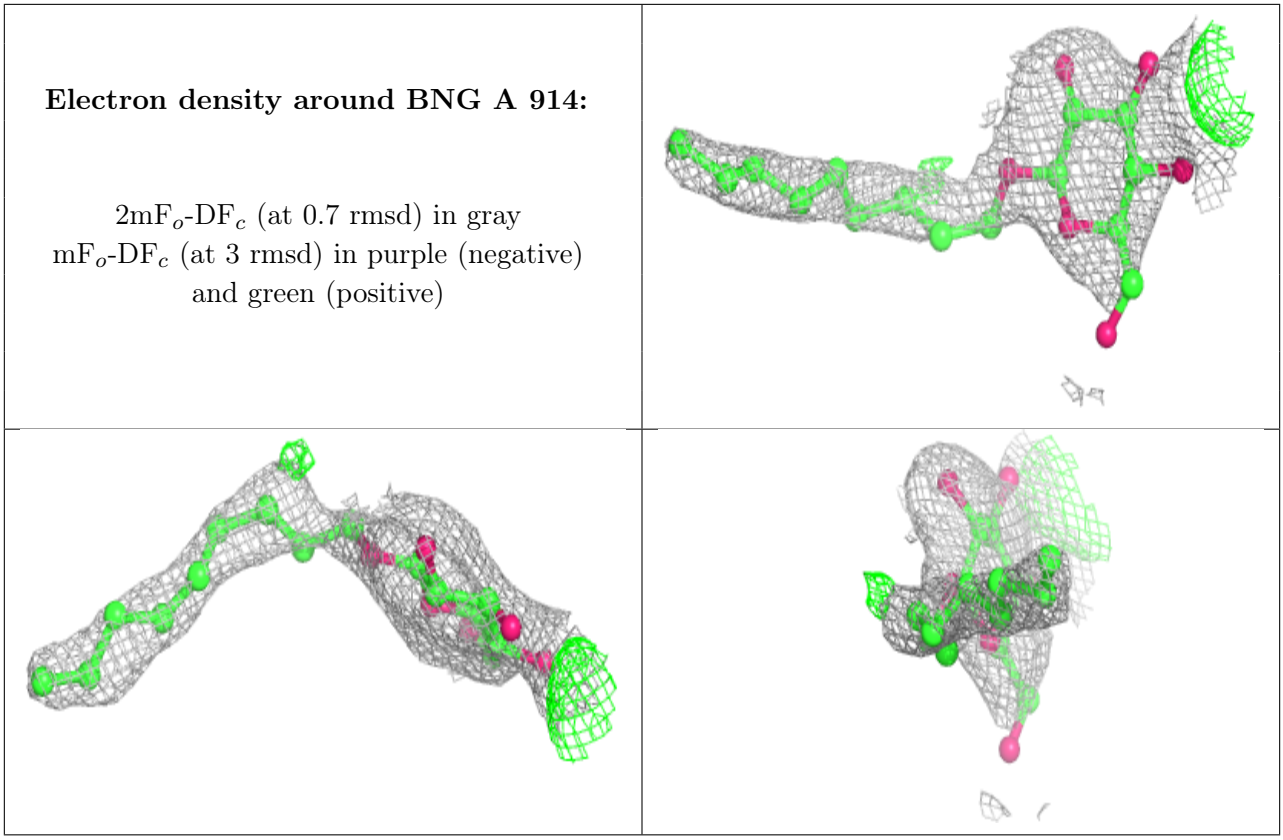
Electron density around BNG A 910:

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



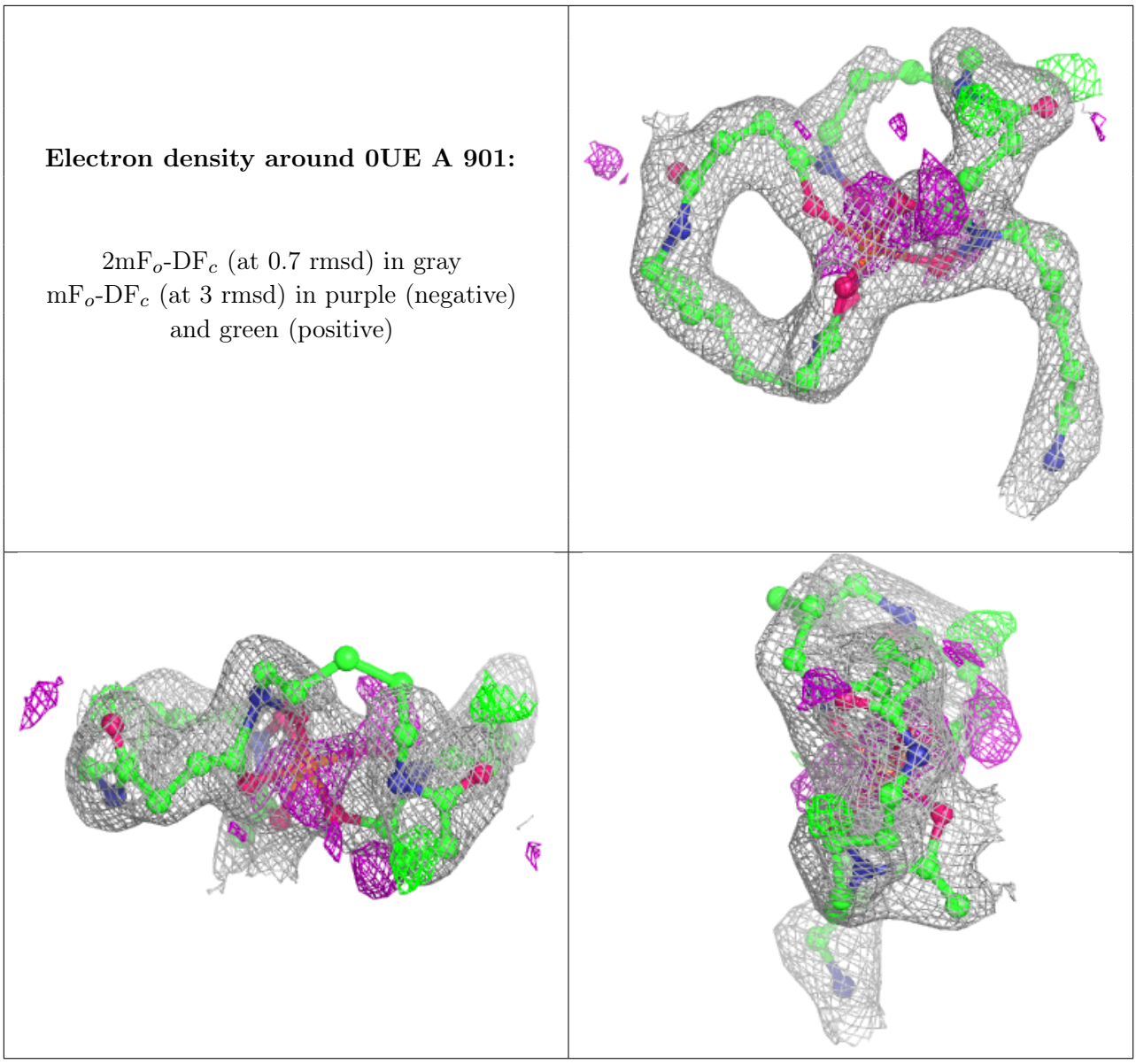
Electron density around BNG A 914:

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



Electron density around 0UE 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)



6.5 Other polymers

There are no such residues in this entry.