



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:37 AM UTC

PDB ID : 8B43 / pdb_00008b43
Title : Crystal structure of ferrioxamine transporter
Authors : Josts, I.; Tidow, H.
Deposited on : 2022-09-19
Resolution : 2.49 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

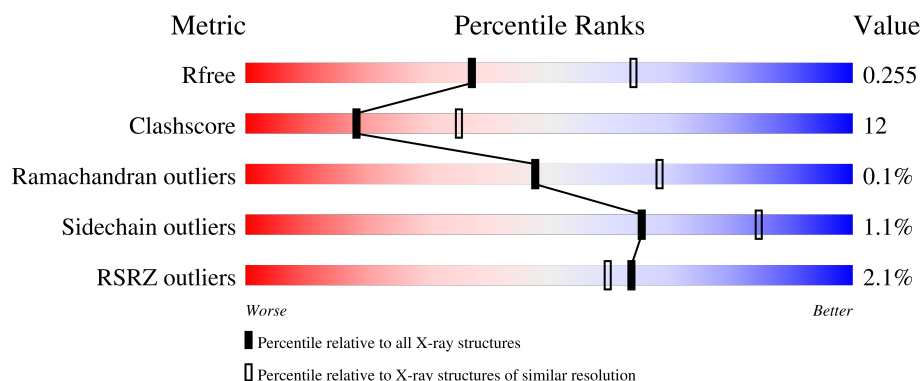
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5457 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 Metal-pseudopaline receptor CntO.

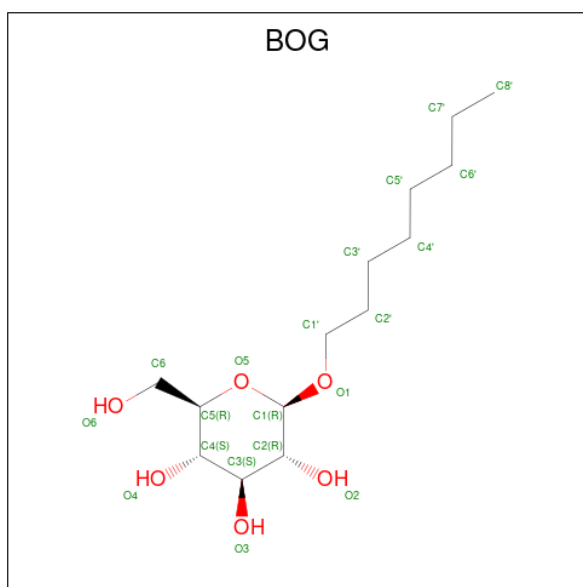
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	677	Total	C	N	O	S	0	0	0
			5324	3345	909	1059	11			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).

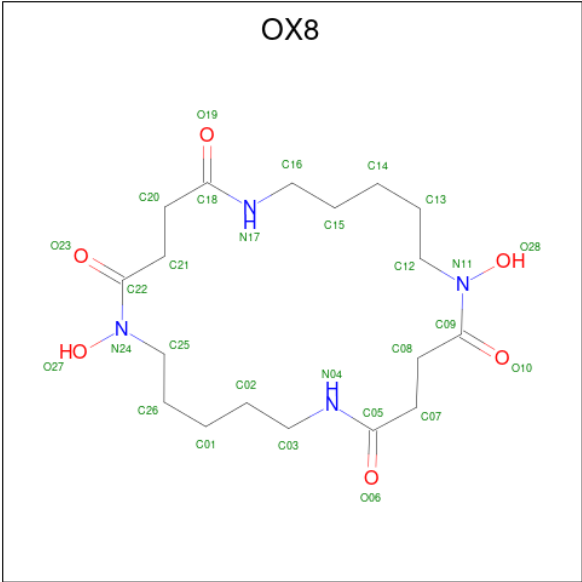


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	8	1		
3	A	1	Total	C	O	0	0
			9	8	1		
3	A	1	Total	C	O	0	0
			9	8	1		

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		

- Molecule 5 is 1,12-bis(oxidanyl)-1,6,12,17-tetrazacyclodocosane-2,5,13,16-tetrone (CCD ID: OX8) (formula: C₁₈H₃₂N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			28	18	4	6		
5	A	1	Total	C	N	O	0	0
			28	18	4	6		
5	A	1	Total	C	N	O	0	0
			28	18	4	6		

- Molecule 1: Metal-pseudopaline receptor CntO



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.41Å 95.41Å 177.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.33 – 2.49 59.33 – 2.49	Depositor EDS
% Data completeness (in resolution range)	62.1 (59.33-2.49) 62.2 (59.33-2.49)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.217 , 0.259 0.217 , 0.255	Depositor DCC
R_{free} test set	994 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5457	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: OX8, SO4, BOG, FE

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	0.58	5/5449 (0.1%)	1.08	36/7393 (0.5%)

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	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	710	HIS	C-N	8.23	1.47	1.33
1	A	652	GLU	CD-OE2	7.85	1.40	1.25
1	A	515	ASN	CA-C	-6.79	1.44	1.52
1	A	304	LYS	CG-CD	6.33	1.71	1.52
1	A	743	ARG	CZ-NH1	5.87	1.41	1.32

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	ASP	N-CA-C	-14.75	89.70	110.35
1	A	380	ASP	CB-CA-C	11.24	127.37	109.61
1	A	514	PHE	CA-C-O	-10.38	109.23	120.24
1	A	799	TYR	CB-CA-C	8.82	128.37	110.38
1	A	332	ASP	CA-C-N	-8.15	105.98	121.54
1	A	332	ASP	C-N-CA	-8.15	105.98	121.54
1	A	639	ASN	CB-CA-C	-8.00	101.08	111.40
1	A	799	TYR	CB-CG-CD2	-7.80	109.10	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	ARG	CB-CG-CD	7.67	128.93	111.30
1	A	478	GLU	CA-CB-CG	7.43	128.96	114.10
1	A	485	ARG	CG-CD-NE	7.10	127.62	112.00
1	A	153	SER	N-CA-C	-6.95	98.85	109.41
1	A	569	ARG	N-CA-CB	-6.61	99.63	110.40
1	A	466	LEU	CB-CG-CD2	6.58	130.44	110.70
1	A	463	ARG	NE-CZ-NH2	6.53	125.07	119.20
1	A	569	ARG	CB-CA-C	6.44	123.46	109.99
1	A	485	ARG	CD-NE-CZ	-6.25	115.65	124.40
1	A	658	GLU	CA-CB-CG	-6.12	101.87	114.10
1	A	810	ARG	N-CA-CB	5.97	118.74	109.48
1	A	569	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	A	577	ASP	CB-CA-C	5.54	119.72	109.70
1	A	793	ASP	N-CA-CB	5.53	119.64	110.47
1	A	339	LYS	CA-CB-CG	5.42	124.94	114.10
1	A	818	TYR	CB-CA-C	5.30	119.27	110.74
1	A	332	ASP	N-CA-C	-5.30	102.91	110.59
1	A	756	LEU	CA-CB-CG	5.20	134.50	116.30
1	A	333	THR	N-CA-C	-5.13	99.88	110.80
1	A	421	ASP	N-CA-CB	-5.12	103.47	111.56
1	A	568	ASN	N-CA-C	-5.12	100.74	108.67
1	A	463	ARG	NE-CZ-NH1	-5.09	116.41	121.50
1	A	550	GLN	CA-CB-CG	5.07	124.24	114.10
1	A	420	ILE	CA-C-N	5.04	130.13	121.87
1	A	420	ILE	C-N-CA	5.04	130.13	121.87
1	A	333	THR	CB-CA-C	-5.03	100.40	110.42
1	A	380	ASP	CA-C-N	5.03	129.88	120.87
1	A	380	ASP	C-N-CA	5.03	129.88	120.87

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	421	ASP	Sidechain
1	A	478	GLU	Sidechain
1	A	637	GLY	Peptide
1	A	639	ASN	Sidechain
1	A	743	ARG	Sidechain
1	A	755	THR	Peptide
1	A	799	TYR	Sidechain
1	A	818	TYR	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	5324	0	5036	127	0
2	A	20	0	0	1	0
3	A	27	0	51	1	0
4	A	2	0	0	0	0
5	A	84	0	0	1	0
All	All	5457	0	5087	128	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 12.

All (128) 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:657:LYS:HE3	1:A:664:TYR:CZ	1.82	1.11
1:A:577:ASP:OD2	1:A:618:PRO:HD2	1.50	1.11
1:A:197:GLN:HB3	1:A:200:ARG:HH11	1.00	1.10
1:A:639:ASN:ND2	1:A:682:GLN:OE1	1.90	1.04
1:A:197:GLN:HB3	1:A:200:ARG:NH1	1.75	1.00
1:A:466:LEU:HD12	1:A:467:GLN:N	1.94	0.83
1:A:788:ASN:O	1:A:810:ARG:HG2	1.78	0.81
1:A:192:SER:OG	1:A:200:ARG:NH2	2.14	0.79
1:A:657:LYS:HE3	1:A:664:TYR:CE2	2.18	0.79
1:A:700:TYR:O	1:A:708:GLN:O	2.00	0.79
1:A:770:TYR:HD2	1:A:772:LEU:HD23	1.47	0.79
1:A:379:ALA:O	1:A:380:ASP:C	2.24	0.78
1:A:200:ARG:HD3	1:A:743:ARG:HH12	1.48	0.78
1:A:703:SER:OG	1:A:705:ASP:OD2	2.01	0.78
1:A:184:ARG:NH1	1:A:256:LEU:O	2.19	0.75
1:A:659:PRO:HD3	1:A:705:ASP:HA	1.68	0.73
1:A:393:ARG:HD3	1:A:793:ASP:OD1	1.89	0.72
1:A:301:MET:HE3	1:A:809:LYS:HD3	1.70	0.71
1:A:758:VAL:HG13	1:A:795:VAL:HG23	1.75	0.67
1:A:381:GLY:HA2	1:A:384:SER:O	1.95	0.67
1:A:152:GLY:CA	1:A:161:HIS:HB2	2.26	0.66
1:A:420:ILE:HG22	1:A:421:ASP:OD2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:LYS:HD3	1:A:521:ASP:HB2	1.78	0.66
1:A:383:LEU:HD21	1:A:795:VAL:HG21	1.79	0.65
1:A:205:ILE:HD11	1:A:261:VAL:HG11	1.78	0.65
1:A:550:GLN:HB2	1:A:590:TYR:CZ	2.32	0.65
1:A:577:ASP:OD2	1:A:618:PRO:CD	2.38	0.65
1:A:770:TYR:CD2	1:A:772:LEU:HD23	2.31	0.64
1:A:167:LYS:HD2	1:A:269:LEU:HD22	1.79	0.64
1:A:197:GLN:CB	1:A:200:ARG:HH11	1.94	0.64
1:A:576:ASP:O	1:A:577:ASP:OD1	2.15	0.64
1:A:292:ARG:O	1:A:819:GLN:HA	1.98	0.63
1:A:658:GLU:HG2	1:A:704:LEU:O	1.99	0.63
1:A:199:MET:HE2	1:A:205:ILE:HD13	1.80	0.62
1:A:627:TRP:CZ2	3:A:905:BOG:H4'2	2.35	0.62
1:A:235:ASP:OD2	1:A:285:LYS:NZ	2.28	0.62
1:A:240:MET:HE3	1:A:470:ILE:HD12	1.82	0.61
1:A:619:LEU:HD23	1:A:666:SER:HB3	1.82	0.61
1:A:657:LYS:HE3	1:A:664:TYR:CE1	2.33	0.61
1:A:200:ARG:HD3	1:A:743:ARG:NH1	2.15	0.59
1:A:773:GLY:HA2	1:A:777:LEU:C	2.29	0.58
1:A:451:GLU:OE1	1:A:454:LYS:HD2	2.03	0.57
1:A:238:LYS:HB3	1:A:240:MET:HE2	1.86	0.57
1:A:187:ILE:HG23	1:A:192:SER:HB2	1.87	0.57
1:A:645:SER:O	1:A:675:LEU:HD12	2.04	0.57
1:A:144:VAL:HG12	1:A:145:PHE:H	1.69	0.56
1:A:581:LYS:NZ	1:A:623:GLU:OE1	2.34	0.56
1:A:717:LYS:NZ	2:A:901:SO4:O3	2.29	0.55
1:A:779:GLY:O	1:A:818:TYR:HA	2.07	0.55
1:A:192:SER:CA	1:A:200:ARG:HH12	2.20	0.55
1:A:192:SER:CB	1:A:200:ARG:HH12	2.21	0.54
1:A:192:SER:HA	1:A:200:ARG:HH12	1.73	0.53
1:A:240:MET:HE1	1:A:495:GLN:CD	2.33	0.53
1:A:366:GLN:HB3	1:A:409:GLN:HG2	1.90	0.53
1:A:192:SER:HA	1:A:200:ARG:NH1	2.25	0.52
1:A:292:ARG:HD2	1:A:820:PHE:HB2	1.92	0.52
1:A:781:ASP:OD1	1:A:817:ASN:HB2	2.10	0.52
1:A:383:LEU:CD2	1:A:795:VAL:HG21	2.40	0.51
1:A:466:LEU:HD12	1:A:466:LEU:C	2.34	0.51
1:A:379:ALA:C	1:A:380:ASP:O	2.41	0.51
1:A:560:ASP:O	1:A:580:GLU:HA	2.10	0.51
1:A:723:TRP:CZ3	1:A:740:GLY:HA2	2.46	0.51
1:A:305:GLU:HB3	1:A:329:LYS:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:GLN:HB2	1:A:590:TYR:CE2	2.46	0.50
1:A:149:ASN:OD1	1:A:427:ARG:NH1	2.44	0.50
1:A:490:THR:HG22	1:A:542:LEU:CD1	2.41	0.50
1:A:612:SER:HA	1:A:618:PRO:HA	1.94	0.49
1:A:330:GLY:HA2	1:A:340:GLU:O	2.12	0.49
1:A:283:SER:O	1:A:285:LYS:HD2	2.13	0.49
1:A:550:GLN:NE2	1:A:591:LEU:O	2.46	0.49
1:A:232:ILE:HD13	1:A:279:VAL:HB	1.95	0.48
1:A:778:LYS:HD2	1:A:779:GLY:H	1.78	0.48
1:A:623:GLU:O	1:A:651:GLN:HA	2.13	0.48
1:A:567:LYS:HD3	1:A:574:LYS:HG2	1.95	0.48
1:A:657:LYS:CE	1:A:664:TYR:CZ	2.76	0.48
1:A:341:GLU:O	1:A:369:PRO:HD2	2.15	0.47
1:A:794:TYR:CZ	1:A:807:GLY:HA3	2.49	0.47
1:A:448:SER:HA	1:A:456:ASN:OD1	2.14	0.47
1:A:604:GLU:HG2	1:A:625:LYS:HG2	1.95	0.47
1:A:271:GLY:HA3	1:A:537:GLN:HE22	1.80	0.47
1:A:738:ILE:CD1	1:A:768:ILE:HD13	2.45	0.47
1:A:201:TYR:OH	1:A:765:ASP:OD2	2.17	0.47
1:A:308:PHE:CE1	1:A:324:LEU:HD23	2.50	0.47
1:A:747:GLU:OE1	1:A:757:ARG:NE	2.49	0.46
1:A:507:SER:OG	1:A:524:SER:HB2	2.14	0.46
1:A:567:LYS:HD3	1:A:574:LYS:CG	2.45	0.46
1:A:537:GLN:HE21	1:A:558:ARG:HH21	1.63	0.46
1:A:292:ARG:O	1:A:819:GLN:HG2	2.17	0.45
1:A:295:THR:HA	1:A:816:VAL:O	2.16	0.45
1:A:335:PHE:O	1:A:338:VAL:HG22	2.17	0.45
1:A:393:ARG:NH2	1:A:793:ASP:OD1	2.30	0.45
1:A:341:GLU:OE2	1:A:343:TYR:OH	2.32	0.45
1:A:485:ARG:HH11	1:A:485:ARG:HD2	1.59	0.45
1:A:152:GLY:HA3	1:A:161:HIS:HB2	1.99	0.45
1:A:238:LYS:HB3	1:A:240:MET:CE	2.46	0.44
1:A:178:THR:HB	1:A:263:LYS:HB2	1.99	0.44
1:A:308:PHE:HE1	1:A:324:LEU:HD23	1.82	0.44
1:A:400:PRO:HD2	1:A:518:TYR:HB3	2.00	0.44
1:A:239:ALA:O	1:A:240:MET:HB2	2.17	0.44
1:A:738:ILE:HD13	1:A:768:ILE:HD13	2.00	0.44
1:A:531:HIS:O	1:A:569:ARG:NH1	2.51	0.44
1:A:749:TRP:CG	1:A:754:ASN:ND2	2.86	0.43
1:A:199:MET:CE	1:A:205:ILE:HD13	2.46	0.43
1:A:271:GLY:HA3	1:A:537:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:SER:OG	1:A:466:LEU:HB3	2.19	0.43
1:A:249:MET:HE1	1:A:435:SER:CB	2.49	0.43
1:A:594:ASN:OD1	1:A:594:ASN:C	2.62	0.43
5:A:910:OX8:O10	5:A:911:OX8:O27	2.37	0.43
1:A:580:GLU:O	1:A:581:LYS:HG2	2.19	0.43
1:A:707:ASN:HA	1:A:710:HIS:ND1	2.34	0.43
1:A:739:GLY:O	1:A:767:ARG:N	2.48	0.43
1:A:657:LYS:HD3	1:A:663:PHE:C	2.45	0.42
1:A:199:MET:HE1	1:A:219:VAL:HG11	2.01	0.42
1:A:657:LYS:CE	1:A:664:TYR:CE1	3.01	0.42
1:A:534:ARG:HB2	1:A:565:THR:OG1	2.19	0.42
1:A:292:ARG:HB2	1:A:820:PHE:HB2	2.01	0.42
1:A:687:LEU:HA	1:A:687:LEU:HD12	1.70	0.42
1:A:543:GLN:HE21	1:A:585:ARG:HH21	1.68	0.41
1:A:752:LYS:HE2	1:A:752:LYS:HB3	1.73	0.41
1:A:761:TYR:HD2	1:A:763:LEU:HD11	1.84	0.41
1:A:687:LEU:HD13	1:A:726:TYR:HD1	1.86	0.41
1:A:210:VAL:HA	1:A:805:TYR:CD2	2.56	0.41
1:A:327:LEU:HD12	1:A:327:LEU:C	2.46	0.41
1:A:265:PRO:HB3	1:A:605:SER:HB3	2.03	0.40
1:A:317:GLU:OE1	1:A:319:ARG:NH1	2.54	0.40
1:A:421:ASP:HB3	1:A:423:VAL:H	1.87	0.40
1:A:197:GLN:O	1:A:200:ARG:NE	2.54	0.40
1:A:206:PHE:HZ	1:A:797:SER:HB3	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	675/820 (82%)	655 (97%)	19 (3%)	1 (0%)	48 68

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	566/667 (85%)	560 (99%)	6 (1%)	65 84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	VAL
1	A	421	ASP
1	A	466	LEU
1	A	499	THR
1	A	615	SER
1	A	682	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	227	ASN
1	A	537	GLN
1	A	543	GLN
1	A	648	HIS
1	A	660	GLN
1	A	673	GLN
1	A	707	ASN
1	A	710	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	BOG	A	906	-	8,8,20	0.76	0	7,7,25	0.84	0
2	SO4	A	912	-	4,4,4	0.25	0	6,6,6	0.10	0
3	BOG	A	905	-	8,8,20	0.75	0	7,7,25	0.72	0
5	OX8	A	911	4	28,28,28	2.72	6 (21%)	26,34,34	1.44	4 (15%)
2	SO4	A	901	-	4,4,4	0.23	0	6,6,6	0.24	0
2	SO4	A	903	-	4,4,4	0.25	0	6,6,6	0.12	0
3	BOG	A	904	-	8,8,20	0.72	0	7,7,25	0.83	0
2	SO4	A	902	-	4,4,4	0.26	0	6,6,6	0.17	0
5	OX8	A	910	4	28,28,28	2.74	6 (21%)	26,34,34	1.54	5 (19%)
5	OX8	A	909	4	28,28,28	2.76	6 (21%)	26,34,34	1.49	7 (26%)

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	BOG	A	906	-	-	1/6/6/31	-
5	OX8	A	911	4	-	14/36/36/36	0/0/1/1
3	BOG	A	905	-	-	1/6/6/31	-
3	BOG	A	904	-	-	3/6/6/31	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OX8	A	910	4	-	9/36/36/36	0/0/1/1
5	OX8	A	909	4	-	11/36/36/36	0/0/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	909	OX8	C09-N11	8.55	1.46	1.35
5	A	911	OX8	C09-N11	8.20	1.46	1.35
5	A	910	OX8	C22-N24	8.18	1.46	1.35
5	A	909	OX8	C22-N24	7.95	1.45	1.35
5	A	910	OX8	C09-N11	7.80	1.45	1.35
5	A	911	OX8	C22-N24	7.70	1.45	1.35
5	A	909	OX8	C18-N17	5.74	1.47	1.33
5	A	911	OX8	C18-N17	5.59	1.46	1.33
5	A	910	OX8	C18-N17	5.37	1.46	1.33
5	A	911	OX8	C05-N04	5.12	1.45	1.33
5	A	909	OX8	C05-N04	4.92	1.45	1.33
5	A	910	OX8	C05-N04	4.81	1.44	1.33
5	A	910	OX8	O06-C05	-2.34	1.18	1.23
5	A	910	OX8	O19-C18	-2.25	1.18	1.23
5	A	909	OX8	O06-C05	-2.17	1.19	1.23
5	A	909	OX8	O19-C18	-2.13	1.19	1.23
5	A	911	OX8	O19-C18	-2.10	1.19	1.23
5	A	911	OX8	O06-C05	-2.09	1.19	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	911	OX8	C20-C18-N17	4.14	123.89	116.34
5	A	910	OX8	C03-N04-C05	-3.88	115.59	122.82
5	A	909	OX8	C08-C07-C05	-3.22	106.04	112.67
5	A	910	OX8	C07-C05-N04	3.05	121.90	116.34
5	A	911	OX8	O27-N24-C25	2.82	120.37	113.76
5	A	910	OX8	O06-C05-N04	-2.73	117.67	123.03
5	A	910	OX8	O28-N11-C12	2.67	120.00	113.76
5	A	909	OX8	O27-N24-C25	2.48	119.58	113.76
5	A	909	OX8	O19-C18-C20	-2.47	117.54	122.02
5	A	911	OX8	O19-C18-C20	-2.44	117.60	122.02
5	A	909	OX8	O28-N11-C12	2.43	119.45	113.76
5	A	909	OX8	C03-N04-C05	-2.41	118.34	122.82
5	A	909	OX8	C07-C05-N04	2.39	120.71	116.34
5	A	911	OX8	O19-C18-N17	-2.30	118.51	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	909	OX8	C16-N17-C18	2.10	126.74	122.82
5	A	910	OX8	C20-C18-N17	2.05	120.07	116.34

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	909	OX8	N11-C12-C13-C14
5	A	909	OX8	C18-C20-C21-C22
5	A	909	OX8	N24-C25-C26-C01
5	A	909	OX8	C13-C12-N11-C09
5	A	909	OX8	C13-C12-N11-O28
5	A	910	OX8	C13-C12-N11-O28
5	A	910	OX8	C26-C25-N24-O27
5	A	911	OX8	N11-C12-C13-C14
5	A	911	OX8	C13-C12-N11-O28
5	A	909	OX8	C15-C16-N17-C18
5	A	911	OX8	C20-C18-N17-C16
5	A	911	OX8	C26-C01-C02-C03
5	A	911	OX8	O19-C18-N17-C16
5	A	911	OX8	C01-C02-C03-N04
5	A	909	OX8	C01-C02-C03-N04
3	A	905	BOG	C1'-C2'-C3'-C4'
5	A	910	OX8	C15-C16-N17-C18
5	A	911	OX8	C02-C01-C26-C25
5	A	909	OX8	C02-C01-C26-C25
5	A	910	OX8	C02-C01-C26-C25
5	A	911	OX8	C12-C13-C14-C15
5	A	911	OX8	C14-C15-C16-N17
3	A	906	BOG	C1'-C2'-C3'-C4'
3	A	904	BOG	O1-C1'-C2'-C3'
5	A	910	OX8	C13-C12-N11-C09
5	A	911	OX8	C18-C20-C21-C22
3	A	904	BOG	C3'-C4'-C5'-C6'
5	A	910	OX8	N24-C25-C26-C01
5	A	909	OX8	C14-C15-C16-N17
5	A	911	OX8	N24-C25-C26-C01
5	A	910	OX8	C07-C08-C09-N11
5	A	911	OX8	C07-C08-C09-N11
3	A	904	BOG	C5'-C6'-C7'-C8'
5	A	909	OX8	O23-C22-N24-O27
5	A	909	OX8	O10-C09-N11-O28

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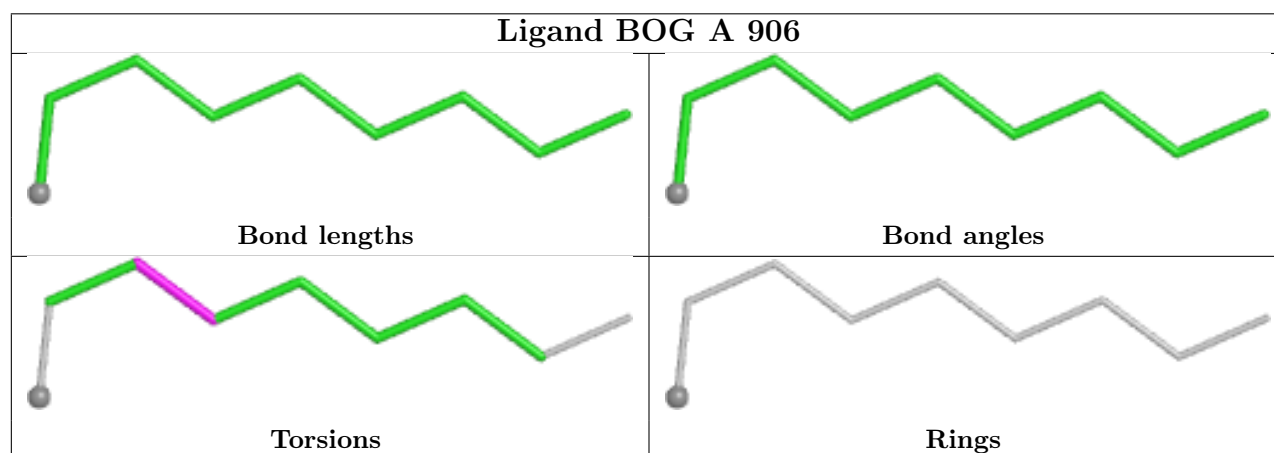
Mol	Chain	Res	Type	Atoms
5	A	910	OX8	O23-C22-N24-O27
5	A	910	OX8	O10-C09-N11-O28
5	A	911	OX8	O23-C22-N24-O27
5	A	911	OX8	O10-C09-N11-O28

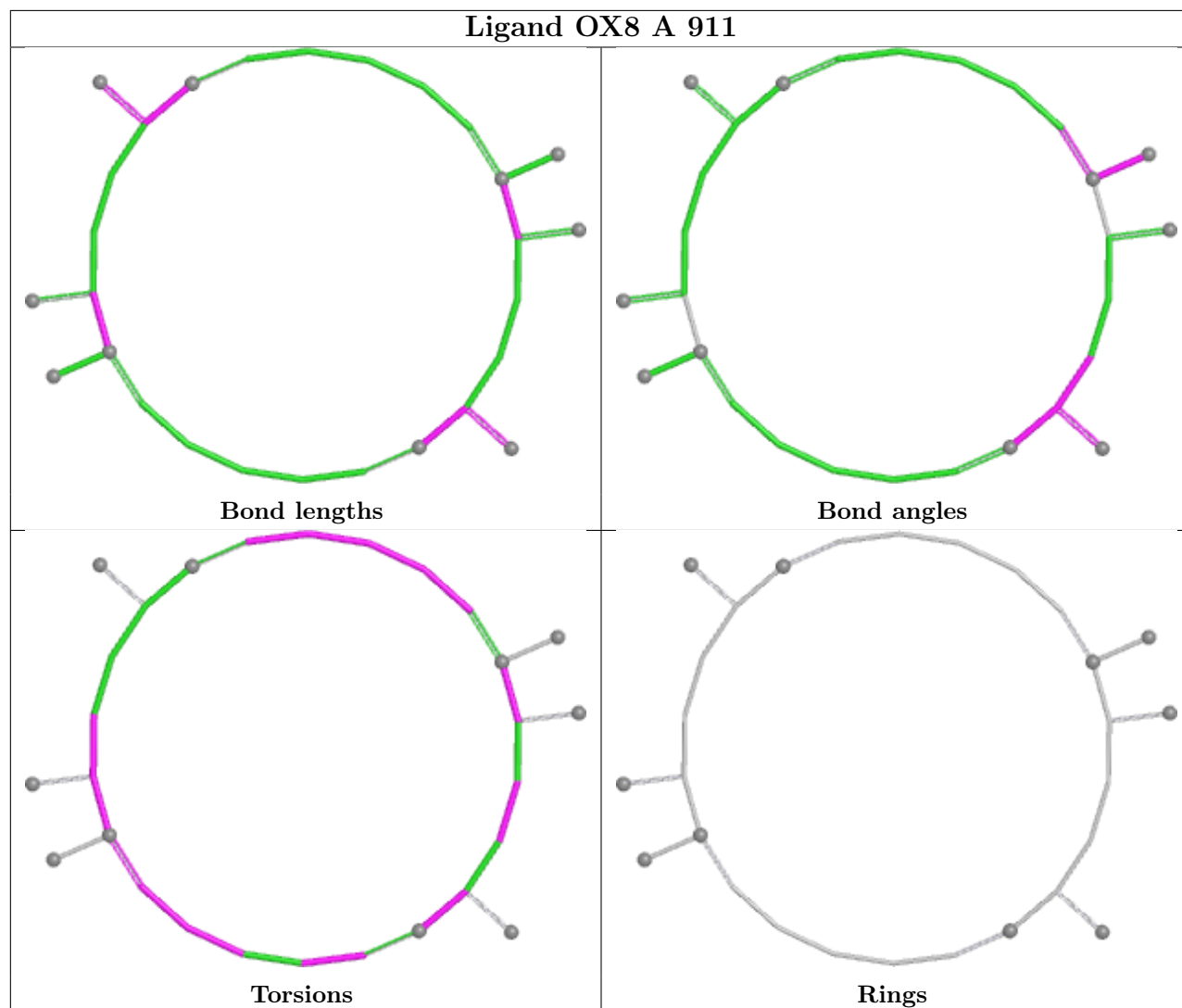
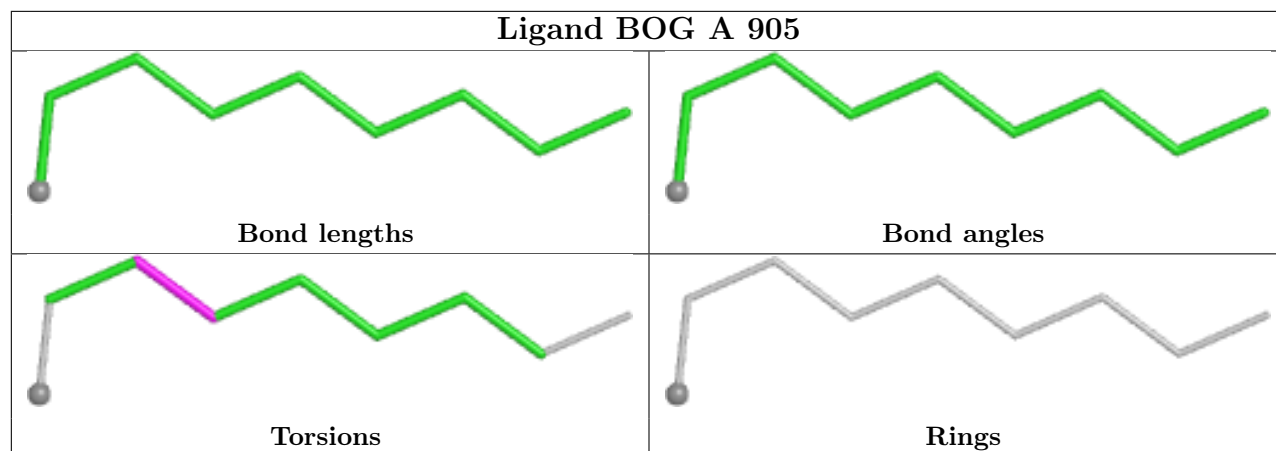
There are no ring outliers.

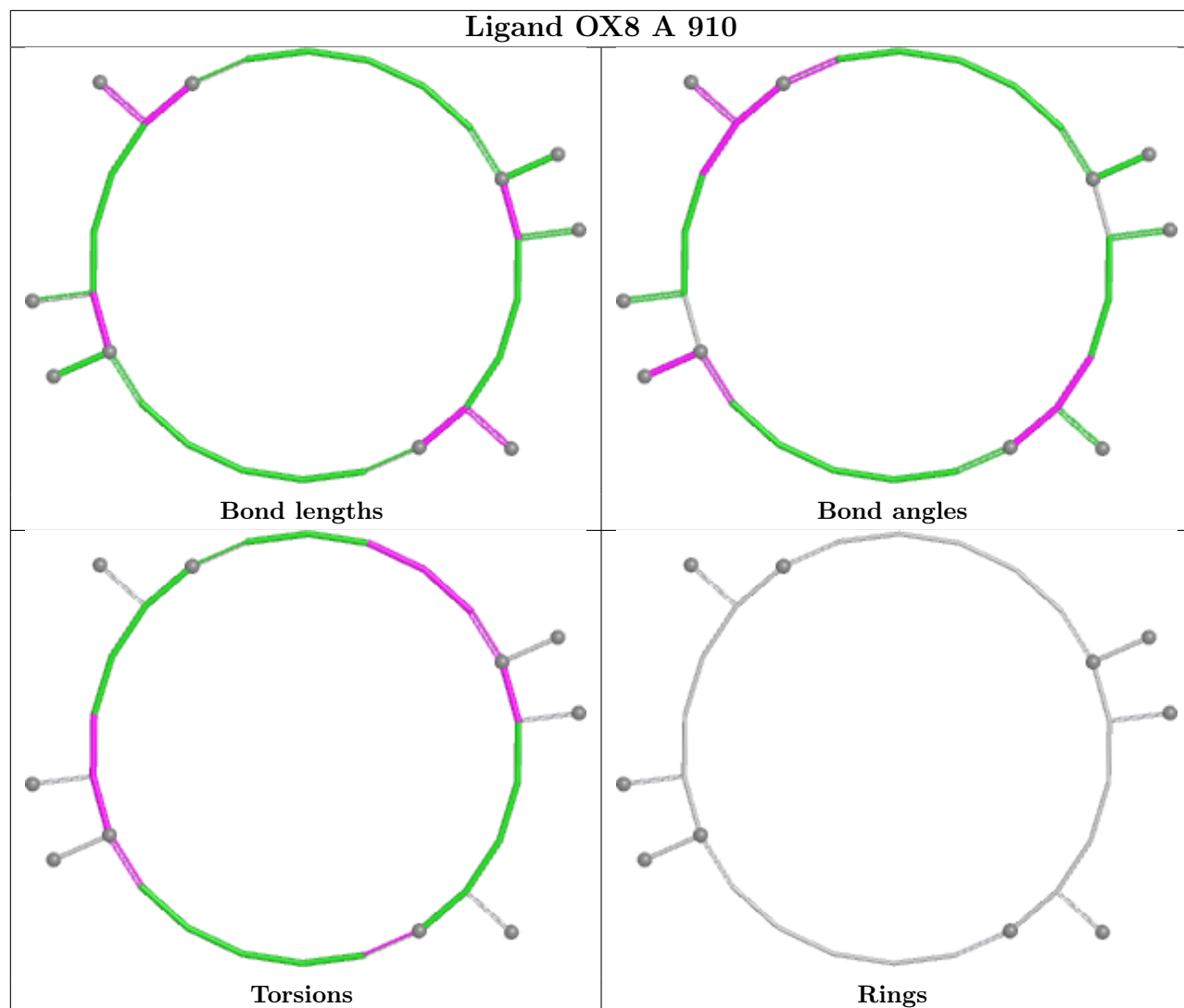
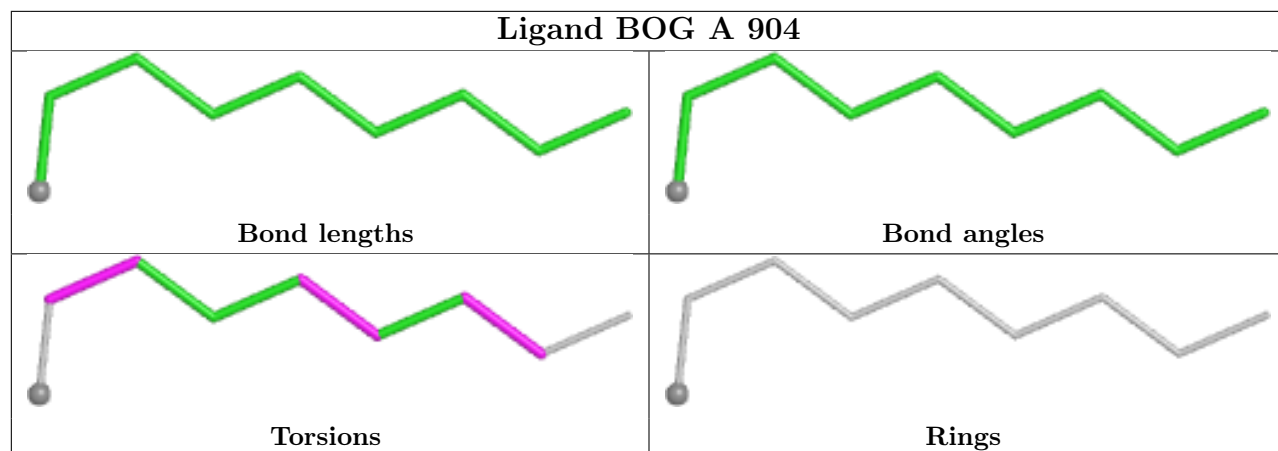
4 monomers are involved in 3 short contacts:

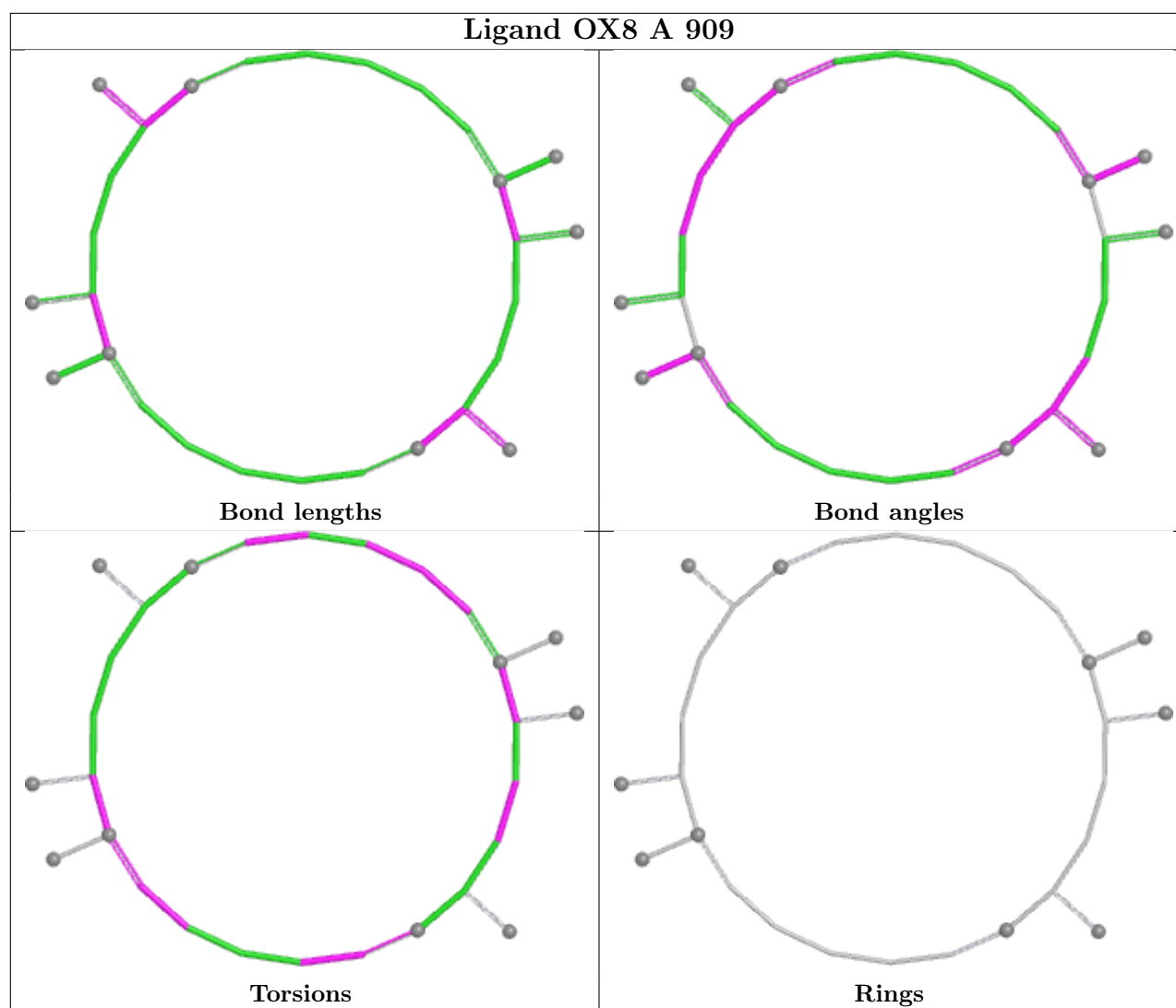
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	905	BOG	1	0
5	A	911	OX8	1	0
2	A	901	SO4	1	0
5	A	910	OX8	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.13	14 (2%) 63 59	32, 57, 93, 123	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	469	TYR	4.1
1	A	799	TYR	3.8
1	A	663	PHE	3.3
1	A	683	LEU	3.2
1	A	395	PHE	3.0
1	A	756	LEU	2.9
1	A	207	THR	2.8
1	A	214	ASN	2.7
1	A	299	GLY	2.7
1	A	275	PRO	2.7
1	A	682	GLN	2.3
1	A	298	ILE	2.2
1	A	200	ARG	2.2
1	A	412	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

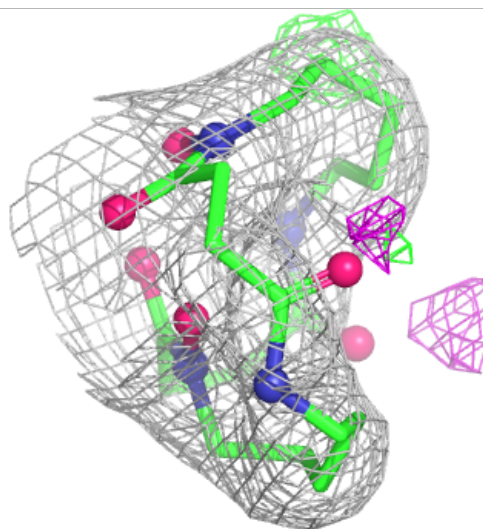
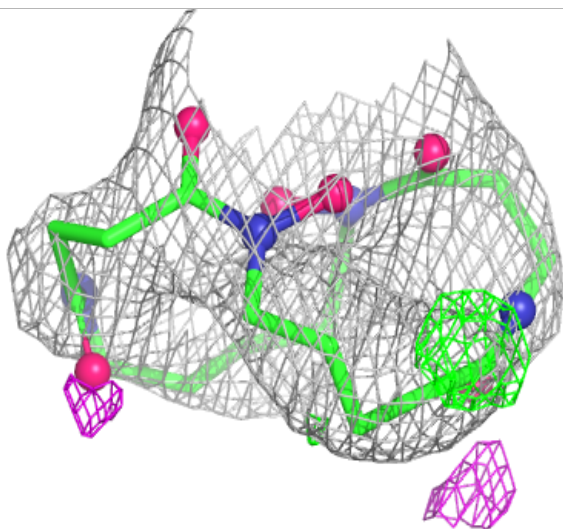
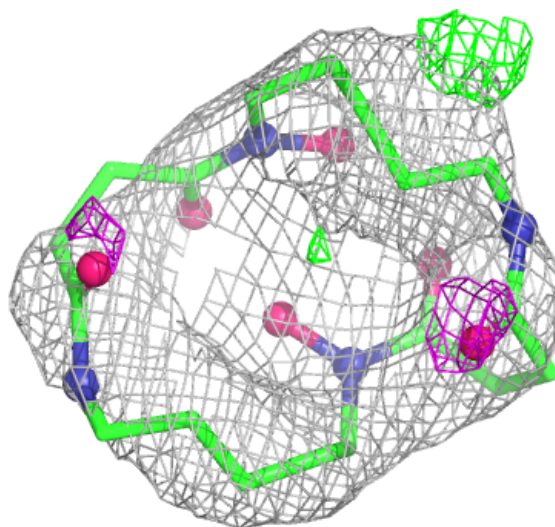
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	912	5/5	0.55	0.11	99,126,139,146	0
2	SO4	A	903	5/5	0.60	0.11	118,131,168,170	0
2	SO4	A	902	5/5	0.79	0.13	63,71,93,96	0
5	OX8	A	909	28/28	0.81	0.15	58,85,100,101	0
3	BOG	A	904	9/20	0.84	0.15	42,49,63,78	0
2	SO4	A	901	5/5	0.84	0.09	85,94,101,104	0
3	BOG	A	906	9/20	0.85	0.14	32,38,48,50	0
3	BOG	A	905	9/20	0.90	0.14	46,52,57,84	0
5	OX8	A	911	28/28	0.91	0.12	33,50,84,92	0
5	OX8	A	910	28/28	0.95	0.10	45,53,61,68	0
4	FE	A	908	1/1	0.99	0.02	70,70,70,70	0
4	FE	A	907	1/1	1.00	0.01	43,43,43,43	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.

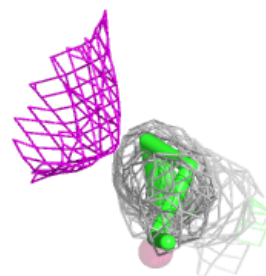
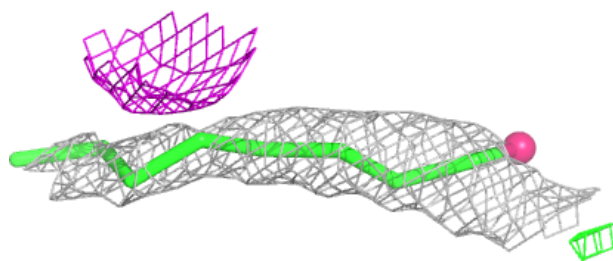
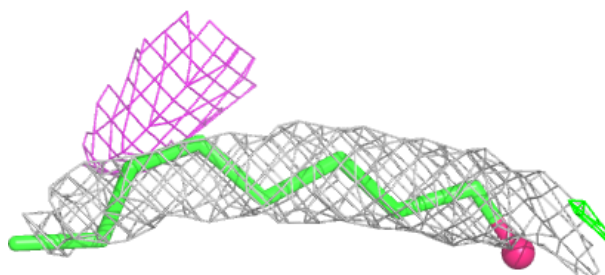
Electron density around OX8 A 909:

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

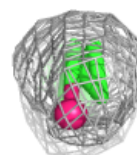
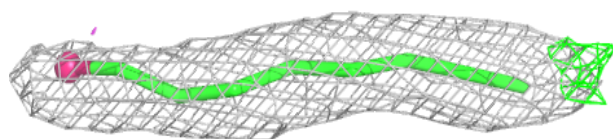
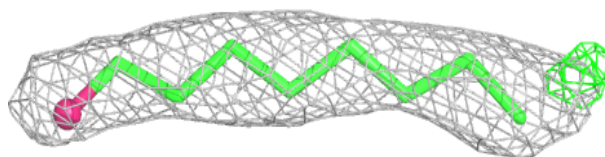


Electron density around BOG A 904:

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

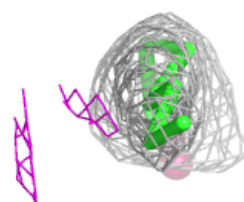
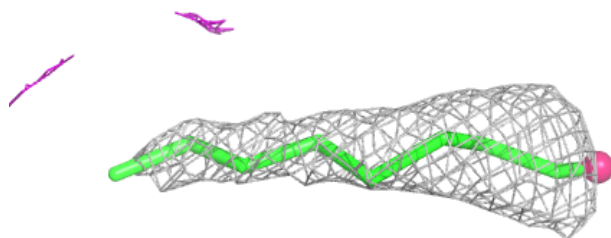
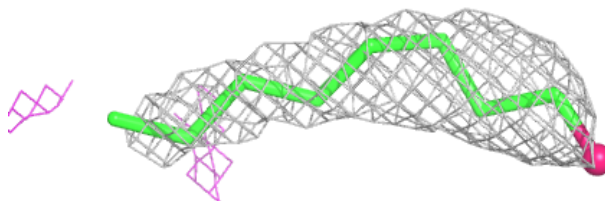
**Electron density around BOG A 906:**

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



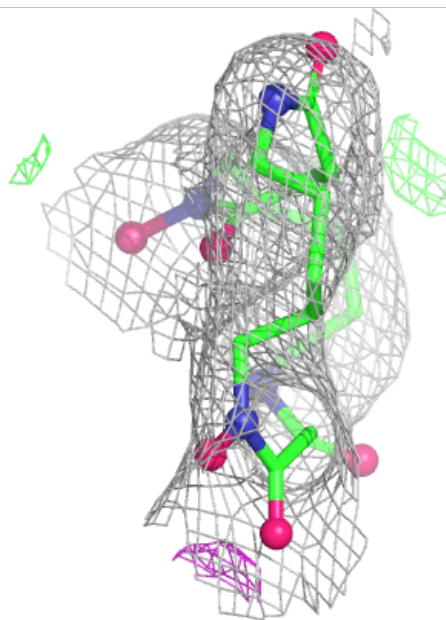
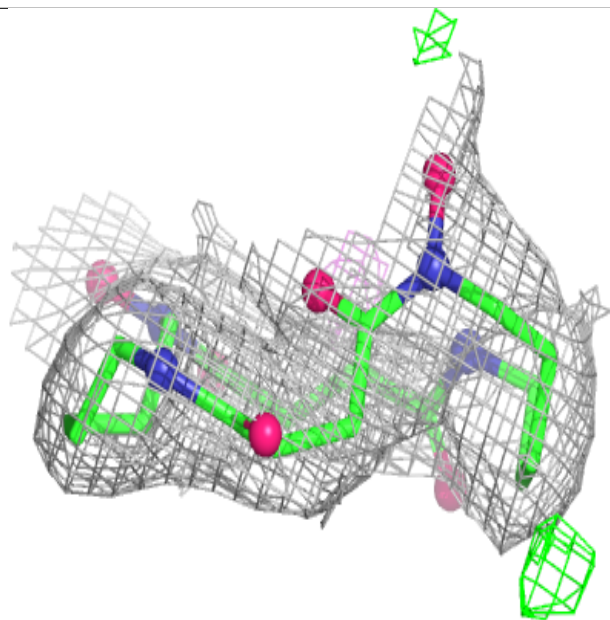
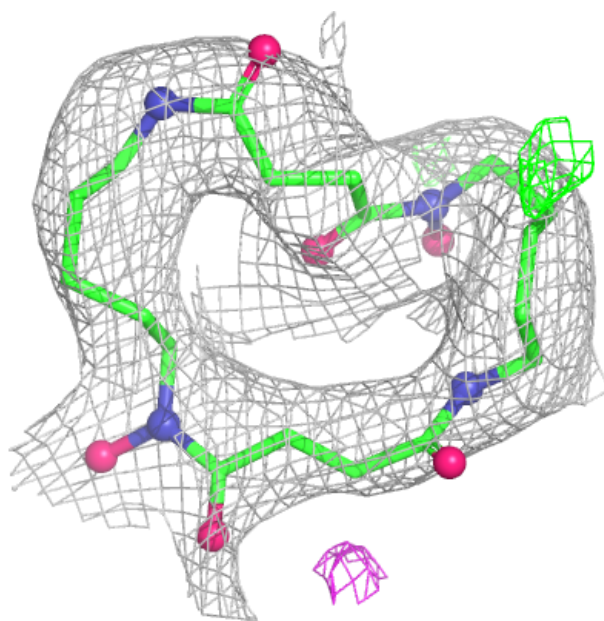
Electron density around BOG A 905:

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



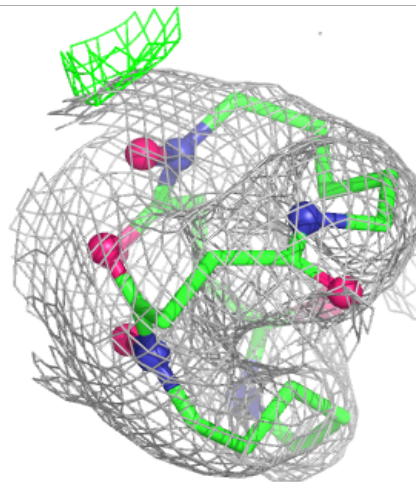
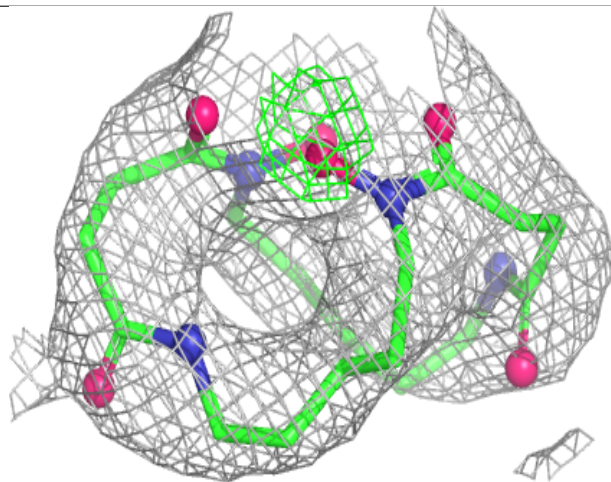
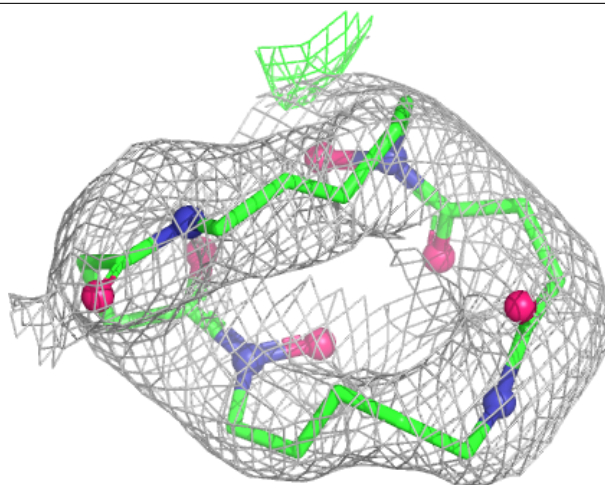
Electron density around OX8 A 911:

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



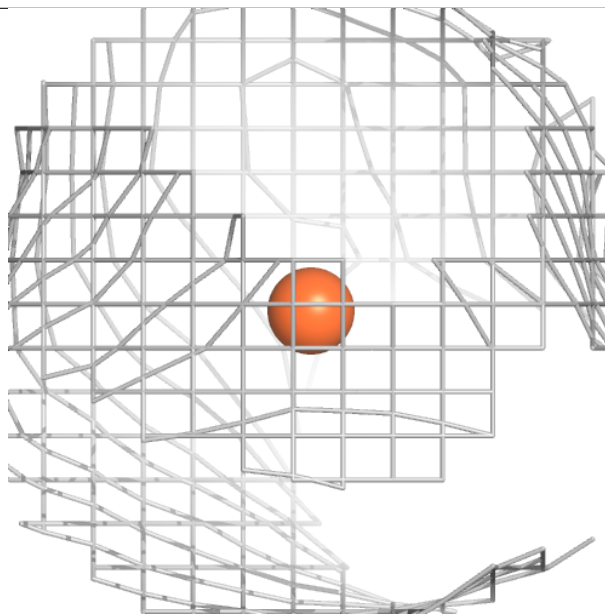
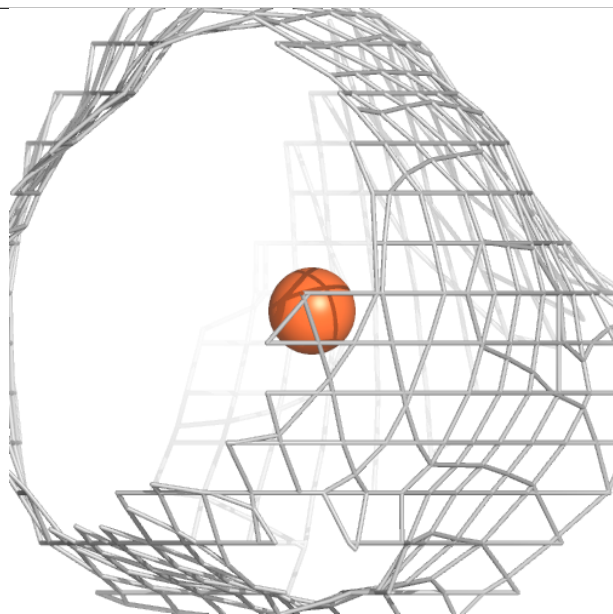
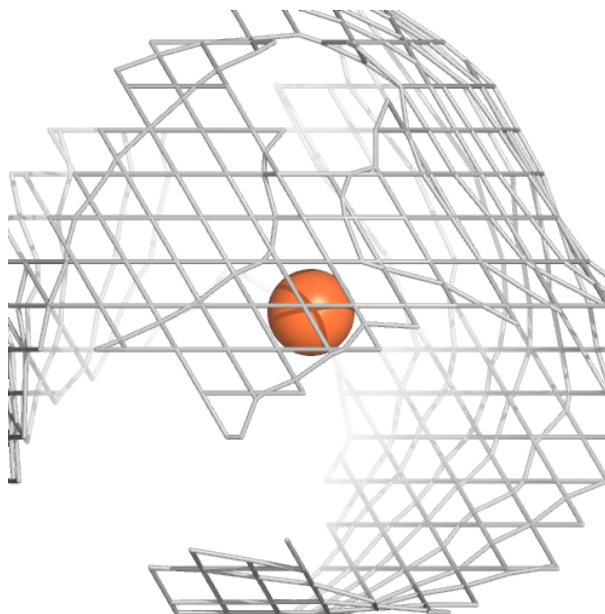
Electron density around OX8 A 910:

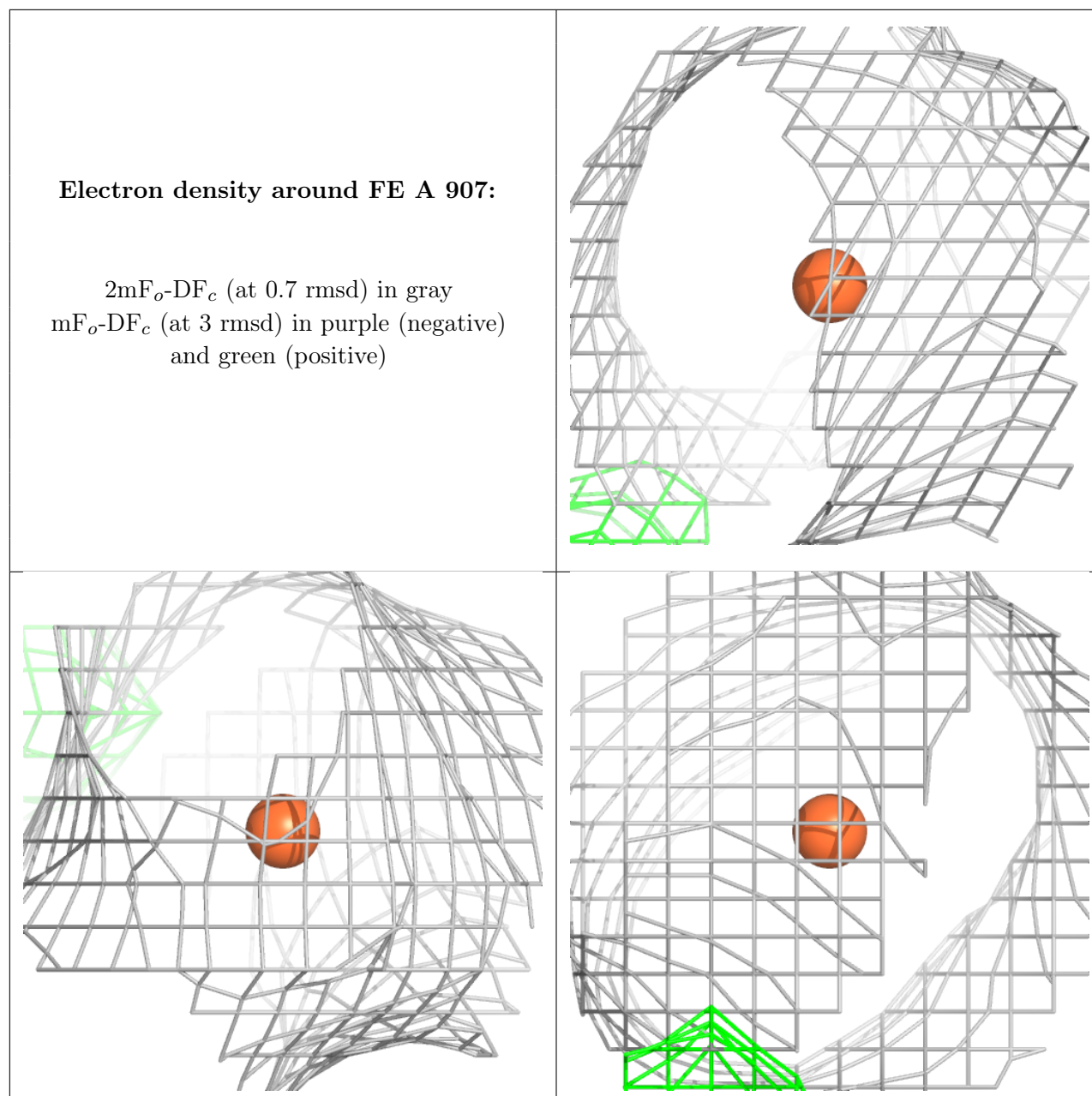
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.