



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:46 AM UTC

PDB ID : 5L3E / pdb_00005l3e
Title : LSD1-CoREST1 in complex with quinazoline-derivative reversible inhibitor
Authors : Speranzini, V.; Rotili, D.; Ciossani, G.; Pilotto, S.; Forgione, M.; Lucidi, A.;
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Deposited on : 2016-04-10
Resolution : 2.80 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

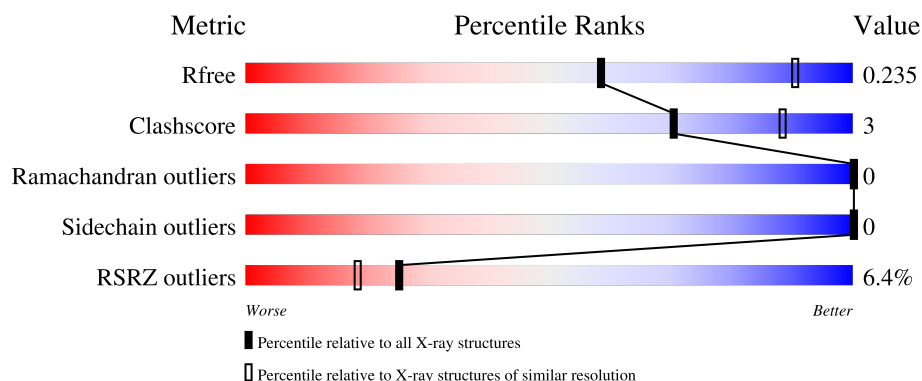
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	730	5% 83% 8% 9%
2	B	178	10% 66% 9% 25%

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
4	E11	A	906	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6522 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.

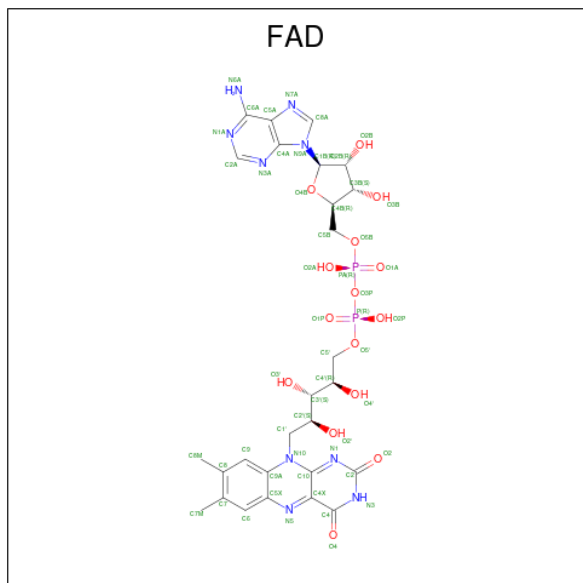
- Molecule 1 is a protein called Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5217	3324	906	967	20			

- Molecule 2 is a protein called REST corepressor 1.

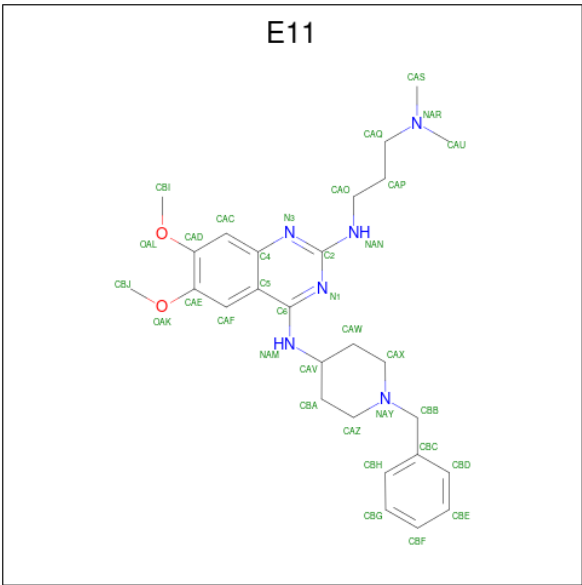
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is N 4 -(1-benzylpiperidin-4-yl)-N 2 -[3-(dimethylamino)propyl]-6,7-dimethoxyquinazoline-2,4-diamine (CCD ID: E11) (formula: $C_{27}H_{38}N_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			35	27	6	2		
4	A	1	Total	C	N	O	0	0
			35	27	6	2		
4	A	1	Total	C	N	O	0	0
			35	27	6	2		
4	A	1	Total	C	N	O	0	0
			35	27	6	2		
4	A	1	Total	C	N	O	0	0
			35	27	6	2		

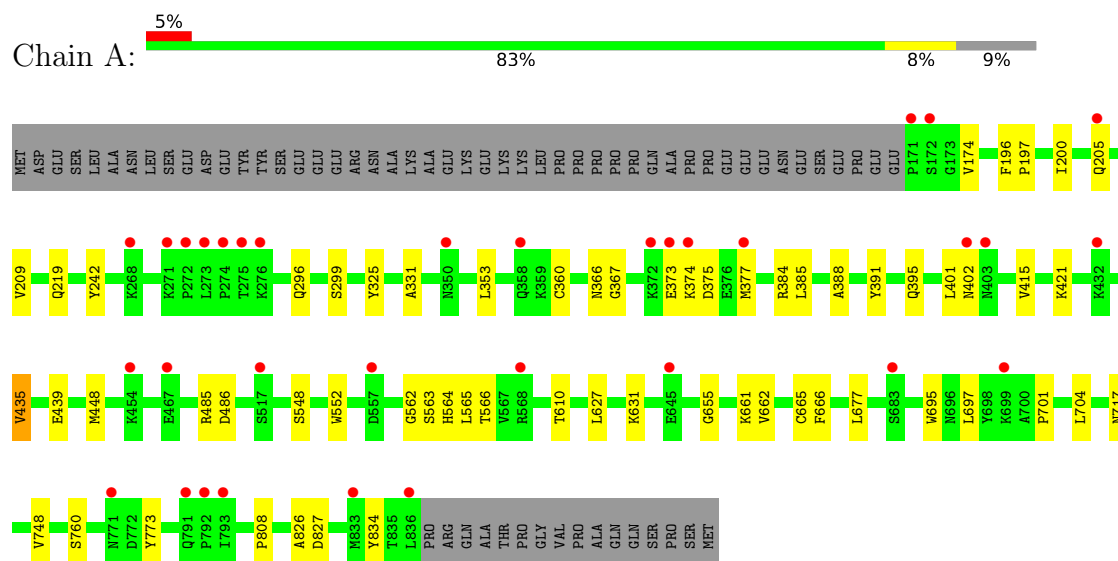
- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

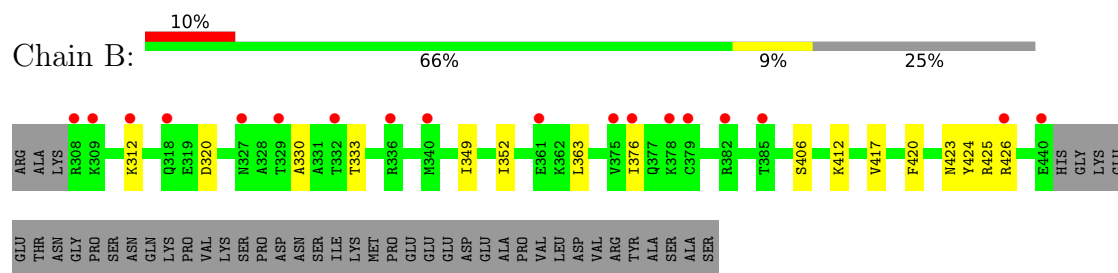
3 Residue-property plots [i](#)

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: Lysine-specific histone demethylase 1A



- Molecule 2: REST corepressor 1



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	116.57Å 178.40Å 233.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.57 – 2.80 98.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (98.57-2.80) 99.7 (98.57-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.200 , 0.224 0.211 , 0.235	Depositor DCC
R_{free} test set	1165 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6522	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: E11, NA, FAD

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	0.94	1/5331 (0.0%)	1.07	4/7232 (0.1%)
2	B	0.78	0/1091	1.00	0/1471
All	All	0.92	1/6422 (0.0%)	1.06	4/8703 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	655	GLY	CA-C	-5.43	1.48	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	610	THR	N-CA-C	6.10	120.57	113.18
1	A	717	ASN	N-CA-C	5.87	120.17	113.19
1	A	834	TYR	N-CA-C	5.66	119.70	112.34
1	A	435	VAL	CB-CA-C	-5.27	105.03	112.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5217	0	5252	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1076	0	1091	11	0
3	A	53	0	31	3	0
4	A	175	0	190	2	0
5	A	1	0	0	0	0
All	All	6522	0	6564	45	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 3.

All (45) 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:353:LEU:HB3	1:A:565:LEU:HD23	1.67	0.77
1:A:562:GLY:O	4:A:904:E11:HAU	1.99	0.62
1:A:661:LYS:HB3	1:A:704:LEU:HD21	1.83	0.61
1:A:564:HIS:C	1:A:565:LEU:HD12	2.28	0.59
1:A:666:PHE:O	1:A:701:PRO:HG2	2.02	0.59
1:A:331:ALA:HA	3:A:901:FAD:N5	2.19	0.56
1:A:391:TYR:CD1	1:A:395:GLN:HG3	2.45	0.52
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.93	0.49
1:A:385:LEU:HD23	1:A:415:VAL:HG12	1.94	0.49
1:A:563:SER:HA	4:A:904:E11:HAS	1.94	0.49
1:A:485:ARG:HG3	1:A:486:ASP:N	2.27	0.48
1:A:325:TYR:CE2	1:A:665:CYS:HB3	2.49	0.48
1:A:385:LEU:O	1:A:388:ALA:HB3	2.13	0.48
1:A:773:TYR:CE2	1:A:808:PRO:HB3	2.48	0.47
1:A:384:ARG:NH2	2:B:312:LYS:O	2.48	0.47
1:A:439:GLU:HG3	2:B:352:ILE:HD13	1.96	0.46
1:A:448:MET:HE2	2:B:363:LEU:HD13	1.96	0.46
1:A:760:SER:HA	3:A:901:FAD:HM81	1.97	0.46
1:A:331:ALA:HA	3:A:901:FAD:C4X	2.45	0.46
2:B:423:ASN:O	2:B:426:ARG:NH1	2.49	0.45
1:A:373:GLU:O	1:A:377:MET:HG2	2.17	0.45
1:A:662:VAL:HG13	1:A:748:VAL:HG22	1.97	0.45
1:A:421:LYS:NZ	2:B:320:ASP:OD1	2.45	0.45
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.82	0.44
1:A:360:CYS:SG	1:A:677:LEU:CD1	3.05	0.44
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.47	0.44
2:B:406:SER:OG	2:B:412:LYS:O	2.34	0.44
1:A:548:SER:O	1:A:552:TRP:HB3	2.17	0.44
1:A:205:GLN:O	1:A:209:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.53	0.43
2:B:376:ILE:HG22	2:B:376:ILE:O	2.18	0.43
1:A:197:PRO:HA	1:A:200:ILE:HG22	2.01	0.43
1:A:826:ALA:O	1:A:827:ASP:C	2.62	0.42
2:B:417:VAL:O	2:B:420:PHE:HB3	2.20	0.42
1:A:401:LEU:O	1:A:402:ASN:HB2	2.20	0.41
1:A:174:VAL:HG12	1:A:219:GLN:OE1	2.20	0.41
1:A:563:SER:O	1:A:565:LEU:CD1	2.69	0.41
1:A:374:LYS:O	1:A:375:ASP:C	2.63	0.41
2:B:424:TYR:O	2:B:425:ARG:C	2.64	0.41
1:A:196:PHE:N	1:A:197:PRO:HD3	2.36	0.41
1:A:296:GLN:O	1:A:299:SER:HB3	2.20	0.41
2:B:330:ALA:HA	2:B:333:THR:HB	2.03	0.41
1:A:366:ASN:OD1	1:A:367:GLY:N	2.54	0.41
1:A:627:LEU:O	1:A:631:LYS:HG3	2.20	0.41
1:A:360:CYS:SG	1:A:677:LEU:HD12	2.62	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	664/730 (91%)	636 (96%)	28 (4%)	0	100	100
2	B	131/178 (74%)	124 (95%)	7 (5%)	0	100	100
All	All	795/908 (88%)	760 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	566/623 (91%)	566 (100%)	0	100	100
2	B	117/156 (75%)	117 (100%)	0	100	100
All	All	683/779 (88%)	683 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	427	GLN
1	A	484	HIS
1	A	535	ASN
1	A	812	HIS
2	B	350	GLN
2	B	411	ASN

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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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
4	E11	A	903	-	37,38,38	1.18	3 (8%)	50,51,51	2.36	17 (34%)
4	E11	A	905	-	37,38,38	1.53	7 (18%)	50,51,51	2.55	16 (32%)
4	E11	A	902	-	37,38,38	1.24	3 (8%)	50,51,51	2.32	20 (40%)
3	FAD	A	901	5	58,58,58	1.48	10 (17%)	85,89,89	1.75	19 (22%)
4	E11	A	904	-	37,38,38	1.37	6 (16%)	50,51,51	2.34	17 (34%)
4	E11	A	906	-	37,38,38	1.31	5 (13%)	50,51,51	2.83	22 (44%)

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
4	E11	A	903	-	-	1/19/29/29	0/4/4/4
4	E11	A	905	-	-	4/19/29/29	0/4/4/4
4	E11	A	902	-	-	0/19/29/29	0/4/4/4
3	FAD	A	901	5	-	3/34/50/50	0/6/6/6
4	E11	A	904	-	-	4/19/29/29	0/4/4/4
4	E11	A	906	-	-	5/19/29/29	0/4/4/4

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	E11	C6-C5	-4.24	1.39	1.44
3	A	901	FAD	C9A-C5X	4.06	1.47	1.41
3	A	901	FAD	C5A-C4A	3.85	1.46	1.39
3	A	901	FAD	C5X-N5	-3.21	1.33	1.39
3	A	901	FAD	C8A-N7A	3.20	1.37	1.31
4	A	906	E11	C6-N1	3.20	1.37	1.33
4	A	905	E11	C6-N1	3.20	1.37	1.33
4	A	904	E11	CAF-CAE	3.09	1.42	1.36
4	A	905	E11	CAC-CAD	2.93	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	905	E11	CBB-CBC	2.85	1.56	1.51
3	A	901	FAD	C4A-N9A	-2.85	1.31	1.37
4	A	905	E11	CAF-CAE	2.83	1.41	1.36
4	A	905	E11	CBB-NAY	2.78	1.52	1.47
4	A	903	E11	C6-N1	2.76	1.36	1.33
3	A	901	FAD	C4-N3	-2.74	1.33	1.38
3	A	901	FAD	C8-C7	2.62	1.47	1.40
3	A	901	FAD	C10-N10	2.61	1.43	1.37
4	A	906	E11	CAF-CAE	2.61	1.41	1.36
3	A	901	FAD	C5A-N7A	-2.57	1.34	1.39
4	A	904	E11	CAC-CAD	2.48	1.41	1.36
4	A	904	E11	C6-N1	2.47	1.36	1.33
4	A	905	E11	C2-NAN	2.44	1.38	1.34
4	A	902	E11	CAF-CAE	2.43	1.41	1.36
3	A	901	FAD	C10-N1	2.42	1.38	1.33
4	A	906	E11	CBB-NAY	2.39	1.52	1.47
4	A	902	E11	CAC-CAD	2.37	1.40	1.36
4	A	903	E11	C6-C5	-2.35	1.41	1.44
4	A	903	E11	CAC-CAD	2.28	1.40	1.36
4	A	904	E11	CAV-NAM	2.24	1.51	1.46
4	A	904	E11	CBB-CBC	2.23	1.55	1.51
4	A	906	E11	C6-C5	-2.17	1.42	1.44
4	A	904	E11	OAK-CAE	2.11	1.40	1.37
4	A	905	E11	OAL-CAD	2.06	1.40	1.37
4	A	906	E11	CBB-CBC	2.01	1.55	1.51

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	905	E11	CBI-OAL-CAD	7.95	129.17	117.51
4	A	904	E11	CBI-OAL-CAD	7.48	128.49	117.51
4	A	902	E11	C6-C5-C4	7.19	120.11	115.86
4	A	903	E11	CBJ-OAK-CAE	7.14	127.99	117.51
4	A	906	E11	OAL-CAD-CAC	-6.90	116.43	125.16
4	A	903	E11	CBI-OAL-CAD	6.78	127.46	117.51
4	A	906	E11	OAL-CAD-CAE	6.24	123.87	115.40
4	A	905	E11	C6-C5-C4	5.77	119.27	115.86
4	A	906	E11	CBC-CBB-NAY	5.44	124.28	113.15
4	A	905	E11	CBJ-OAK-CAE	5.40	125.44	117.51
4	A	902	E11	CAF-C5-C6	-5.37	120.47	124.84
4	A	904	E11	CBJ-OAK-CAE	5.35	125.36	117.51
4	A	903	E11	CAW-CAV-NAM	-5.31	102.22	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	906	E11	OAK-CAE-CAF	-5.28	118.48	125.16
4	A	905	E11	CBC-CBB-NAY	5.20	123.78	113.15
4	A	902	E11	CBJ-OAK-CAE	5.17	125.10	117.51
4	A	904	E11	C6-C5-C4	5.14	118.89	115.86
4	A	906	E11	OAK-CAE-CAD	5.02	122.22	115.40
4	A	903	E11	N3-C2-N1	-4.96	118.12	126.25
3	A	901	FAD	N3A-C2A-N1A	-4.88	121.20	128.58
4	A	905	E11	N3-C2-N1	-4.80	118.40	126.25
4	A	906	E11	CBA-CAV-NAM	-4.74	103.14	110.77
4	A	906	E11	CAW-CAX-NAY	4.74	118.74	111.08
4	A	905	E11	CBA-CAZ-NAY	4.71	118.69	111.08
4	A	904	E11	N3-C2-N1	-4.58	118.76	126.25
4	A	906	E11	CBJ-OAK-CAE	4.55	124.18	117.51
4	A	906	E11	N3-C2-N1	-4.28	119.24	126.25
3	A	901	FAD	C5'-C4'-C3'	-4.25	104.19	112.22
4	A	906	E11	CAX-CAW-CAV	4.08	117.12	110.67
4	A	902	E11	CBI-OAL-CAD	4.06	123.47	117.51
4	A	904	E11	C5-C6-N1	-3.87	116.27	122.07
4	A	906	E11	CAZ-NAY-CAX	3.84	117.11	108.84
3	A	901	FAD	O4-C4-C4X	-3.83	116.42	126.53
4	A	902	E11	OAK-CAE-CAF	-3.78	120.37	125.16
4	A	903	E11	NAN-C2-N3	3.76	123.64	117.16
4	A	905	E11	C2-N3-C4	3.73	121.45	115.54
4	A	902	E11	C5-C6-N1	-3.73	116.48	122.07
4	A	903	E11	C2-N3-C4	3.70	121.41	115.54
4	A	904	E11	C2-N3-C4	3.64	121.32	115.54
3	A	901	FAD	C5A-C4A-N3A	-3.61	121.75	126.72
4	A	902	E11	CAW-CAX-NAY	3.60	116.90	111.08
3	A	901	FAD	C4'-C3'-C2'	-3.60	107.58	113.57
4	A	905	E11	CAZ-NAY-CAX	3.60	116.59	108.84
4	A	903	E11	C6-C5-C4	3.55	117.96	115.86
4	A	904	E11	C2-N1-C6	3.52	125.01	116.36
4	A	906	E11	NAN-C2-N3	3.46	123.12	117.16
3	A	901	FAD	N3A-C4A-N9A	3.43	133.01	127.17
4	A	904	E11	OAK-CAE-CAF	-3.39	120.87	125.16
4	A	906	E11	CBI-OAL-CAD	3.26	122.30	117.51
3	A	901	FAD	C2A-N3A-C4A	3.26	119.80	111.83
4	A	905	E11	CAW-CAX-NAY	3.26	116.35	111.08
4	A	906	E11	CAO-NAN-C2	3.26	129.46	123.82
3	A	901	FAD	C4A-N9A-C1B	-3.23	119.08	126.63
4	A	905	E11	C5-C4-N3	-3.23	119.38	122.80
4	A	902	E11	OAL-CAD-CAE	3.21	119.76	115.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	903	E11	C2-N1-C6	3.19	124.19	116.36
4	A	905	E11	C2-N1-C6	3.17	124.15	116.36
4	A	903	E11	CAF-C5-C6	-3.17	122.26	124.84
4	A	906	E11	C2-N3-C4	3.16	120.55	115.54
4	A	905	E11	C5-C6-N1	-3.15	117.35	122.07
4	A	905	E11	CAF-C5-C6	-3.14	122.28	124.84
4	A	904	E11	NAN-C2-N3	3.07	122.45	117.16
4	A	902	E11	C2-N1-C6	3.00	123.74	116.36
4	A	906	E11	CAP-CAO-NAN	-2.98	103.41	111.46
3	A	901	FAD	C4A-N9A-C8A	2.97	108.85	105.74
4	A	902	E11	CAO-NAN-C2	-2.96	118.69	123.82
4	A	902	E11	N3-C2-N1	-2.95	121.43	126.25
4	A	902	E11	CAU-NAR-CAS	2.89	117.13	109.72
4	A	902	E11	OAL-CAD-CAC	-2.89	121.50	125.16
4	A	904	E11	C5-C4-N3	-2.88	119.75	122.80
4	A	905	E11	CBA-CAV-CAW	-2.86	105.86	110.80
4	A	902	E11	OAK-CAE-CAD	2.81	119.21	115.40
4	A	904	E11	OAK-CAE-CAD	2.80	119.21	115.40
4	A	904	E11	CBC-CBB-NAY	2.78	118.84	113.15
3	A	901	FAD	C2A-N1A-C6A	2.73	123.22	118.73
4	A	905	E11	NAN-C2-N3	2.71	121.83	117.16
4	A	903	E11	C5-C6-N1	-2.67	118.07	122.07
4	A	906	E11	C2-N1-C6	2.65	122.88	116.36
4	A	906	E11	C6-C5-C4	2.58	117.38	115.86
3	A	901	FAD	C4X-C10-N1	-2.57	118.28	124.59
3	A	901	FAD	C4X-C4-N3	2.54	119.72	113.25
4	A	904	E11	CAP-CAO-NAN	-2.52	104.65	111.46
4	A	906	E11	CBB-NAY-CAX	2.48	116.41	111.07
3	A	901	FAD	O2A-PA-O3P	2.48	113.98	107.27
3	A	901	FAD	O2P-P-O1P	2.47	123.95	112.44
3	A	901	FAD	N10-C10-N1	2.46	125.75	118.51
4	A	902	E11	NAN-C2-N3	2.44	121.37	117.16
4	A	903	E11	CAZ-NAY-CAX	2.43	114.08	108.84
4	A	903	E11	C5-C4-N3	-2.41	120.25	122.80
4	A	906	E11	CBB-CBC-CBH	2.41	125.19	120.75
3	A	901	FAD	C5A-C6A-N6A	-2.37	117.42	123.29
3	A	901	FAD	O5'-P-O1P	-2.34	99.65	108.94
4	A	906	E11	C5-C6-N1	-2.31	118.61	122.07
4	A	903	E11	CBH-CBC-CBD	2.28	121.62	118.23
4	A	904	E11	CAW-CAV-NAM	2.21	114.33	110.77
4	A	902	E11	CAP-CAO-NAN	-2.20	105.51	111.46
4	A	902	E11	CAZ-CBA-CAV	2.18	114.11	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	FAD	N6A-C6A-N1A	2.18	123.22	118.38
3	A	901	FAD	C1B-N9A-C8A	2.16	131.89	127.09
4	A	903	E11	CBF-CBG-CBH	-2.16	117.58	120.24
4	A	903	E11	CBG-CBF-CBE	2.15	122.81	119.87
4	A	902	E11	C5-C4-N3	-2.15	120.53	122.80
4	A	904	E11	CAU-NAR-CAS	2.15	115.22	109.72
4	A	902	E11	CBB-NAY-CAZ	2.14	115.67	111.07
4	A	904	E11	CAZ-CBA-CAV	2.13	114.04	110.67
4	A	904	E11	CAF-C5-C6	-2.13	123.11	124.84
4	A	905	E11	CAZ-CBA-CAV	2.13	114.03	110.67
4	A	902	E11	CAW-CAV-NAM	-2.10	107.40	110.77
4	A	903	E11	CBA-CAV-NAM	2.09	114.14	110.77
4	A	906	E11	CBB-NAY-CAZ	2.05	115.48	111.07
4	A	903	E11	C6-NAM-CAV	-2.01	120.55	124.06

There are no chirality outliers.

All (17) torsion outliers are listed below:

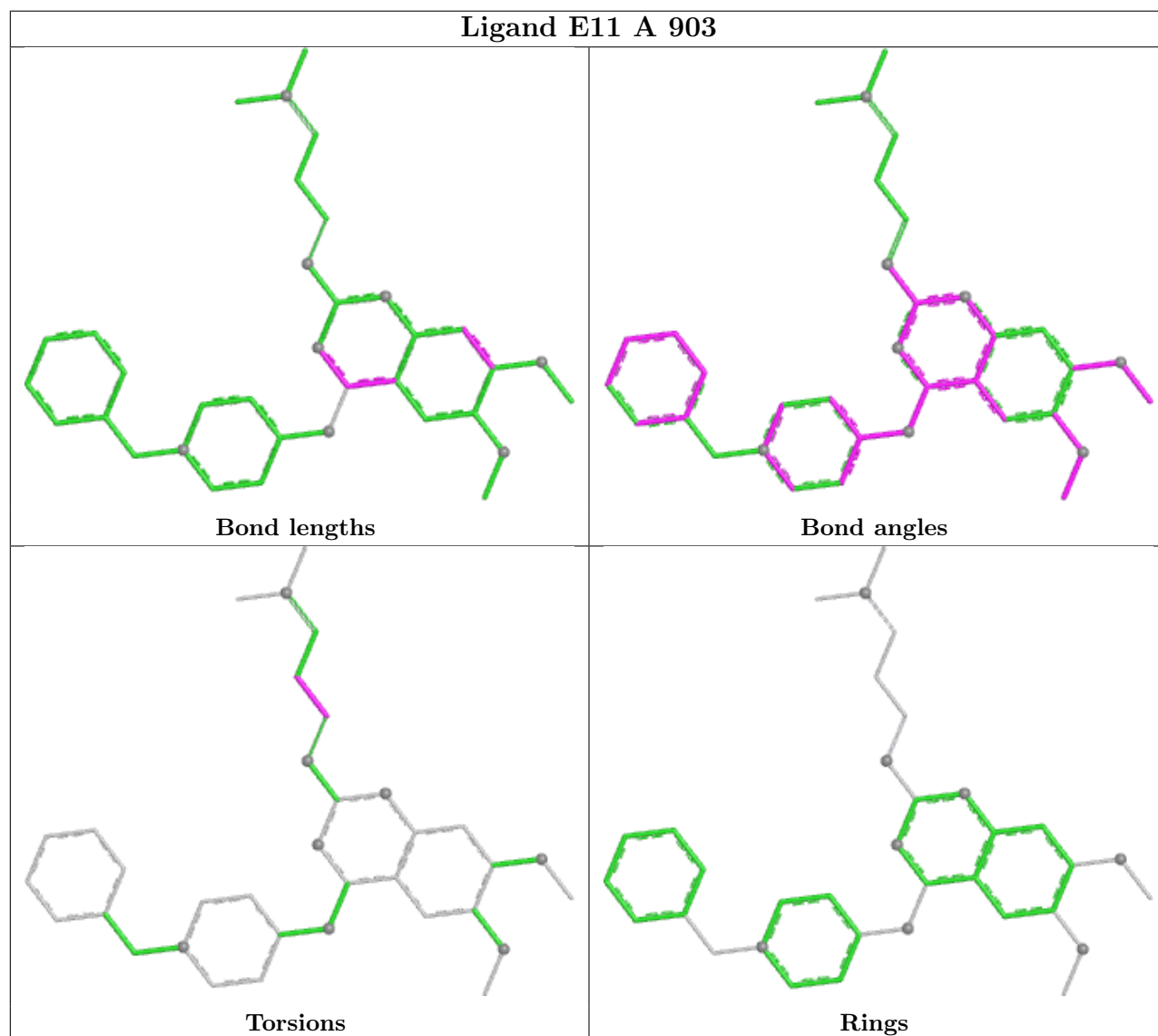
Mol	Chain	Res	Type	Atoms
4	A	906	E11	CAD-CAE-OAK-CBJ
4	A	906	E11	CAE-CAD-OAL-CBI
4	A	906	E11	CAC-CAD-OAL-CBI
4	A	906	E11	CAF-CAE-OAK-CBJ
4	A	905	E11	CAO-CAP-CAQ-NAR
4	A	904	E11	CAD-CAE-OAK-CBJ
4	A	904	E11	CAF-CAE-OAK-CBJ
3	A	901	FAD	PA-O3P-P-O5'
4	A	906	E11	CAO-CAP-CAQ-NAR
3	A	901	FAD	C2'-C3'-C4'-O4'
4	A	904	E11	CAE-CAD-OAL-CBI
4	A	905	E11	CAD-CAE-OAK-CBJ
4	A	903	E11	NAN-CAO-CAP-CAQ
4	A	904	E11	CAC-CAD-OAL-CBI
4	A	905	E11	CAP-CAO-NAN-C2
3	A	901	FAD	O4B-C4B-C5B-O5B
4	A	905	E11	CAF-CAE-OAK-CBJ

There are no ring outliers.

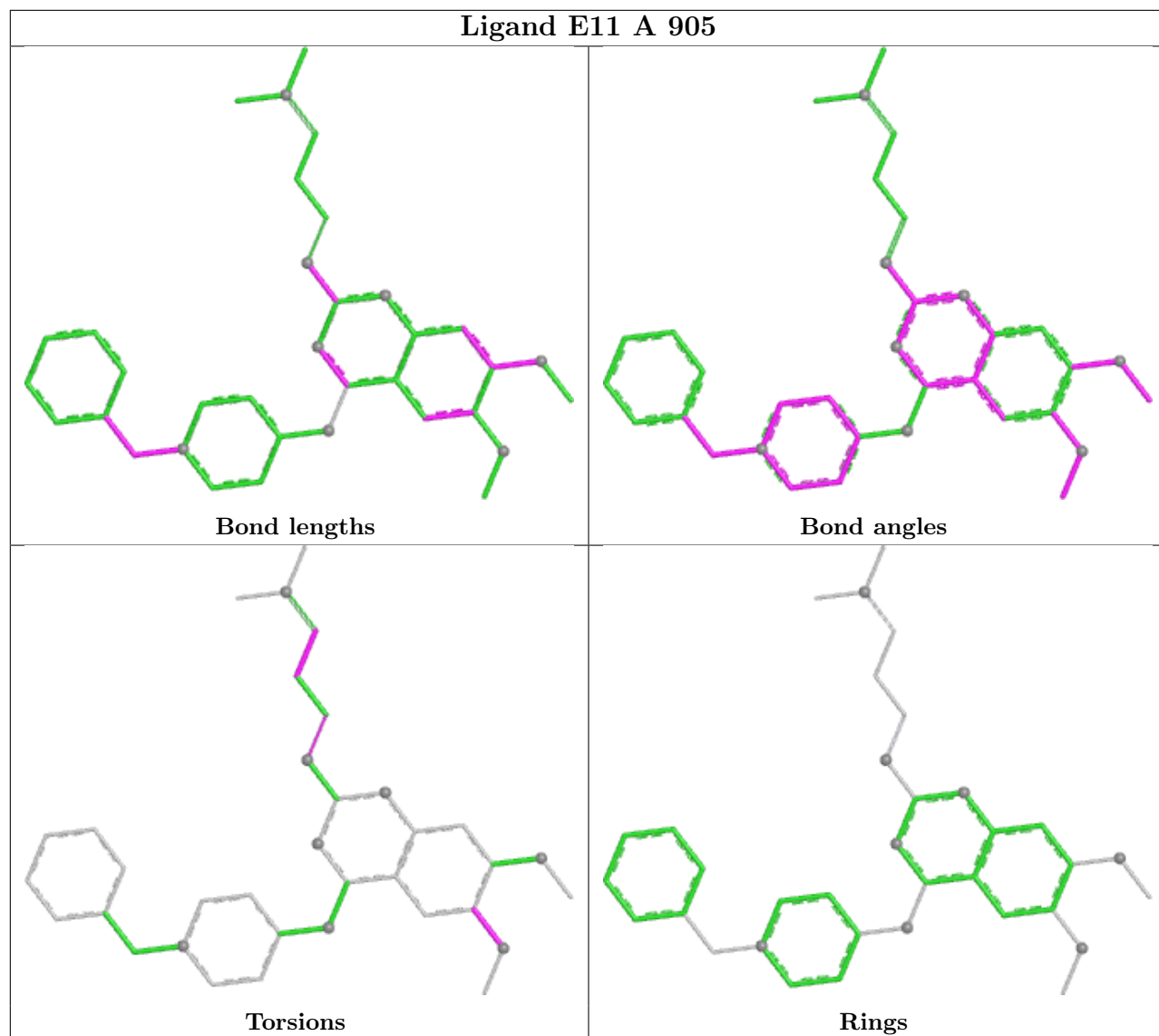
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	FAD	3	0
4	A	904	E11	2	0

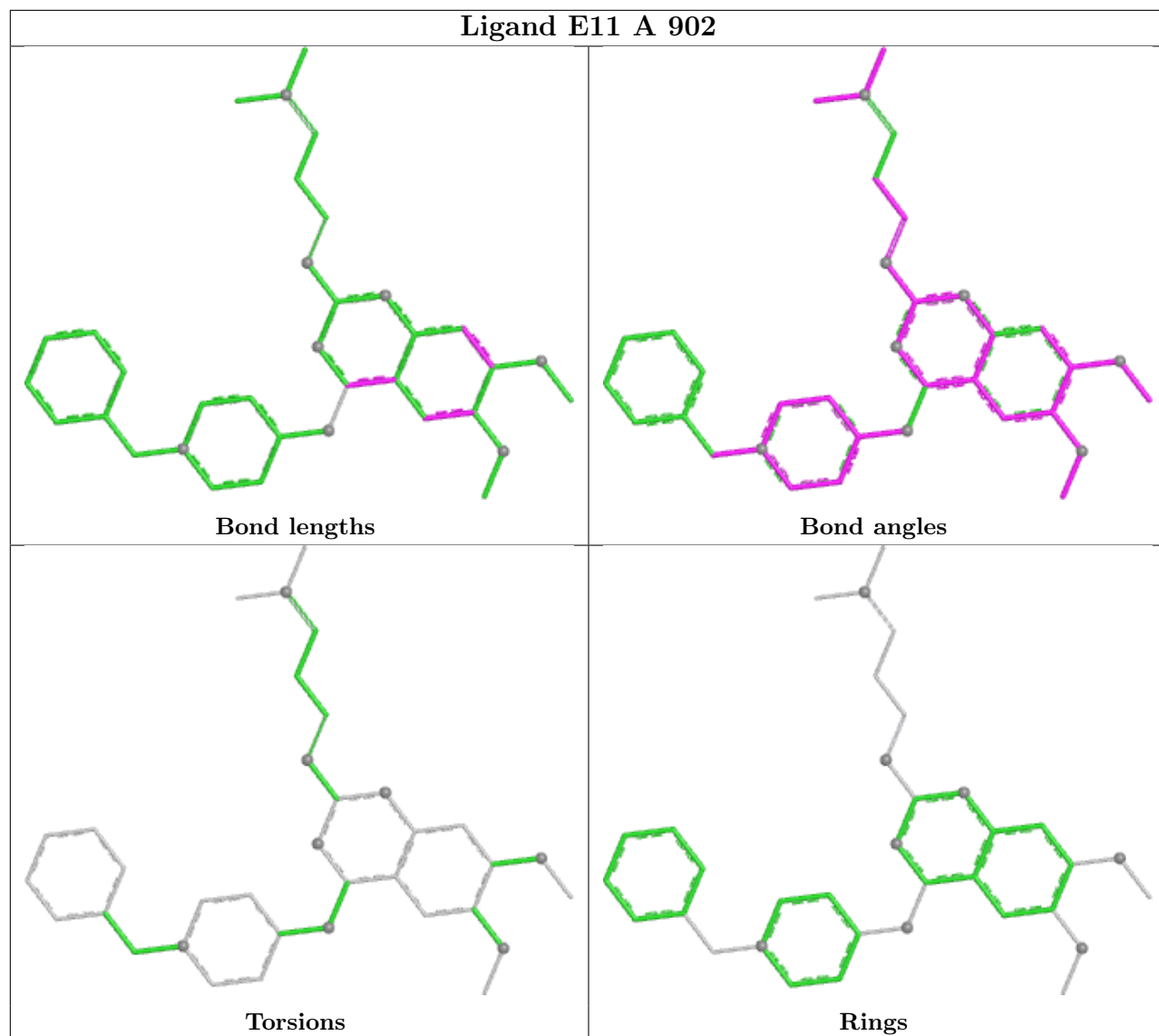
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

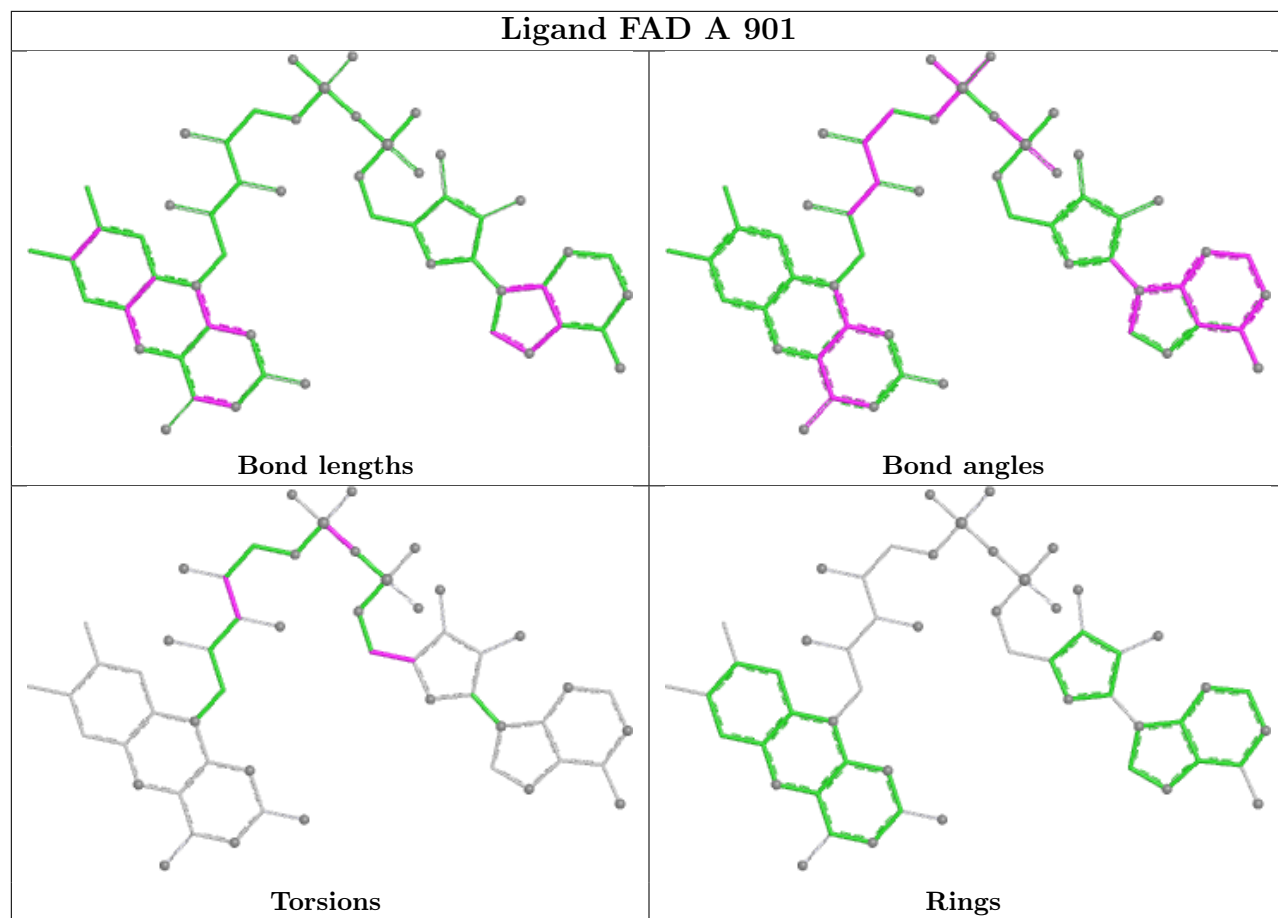


Ligand E11 A 905

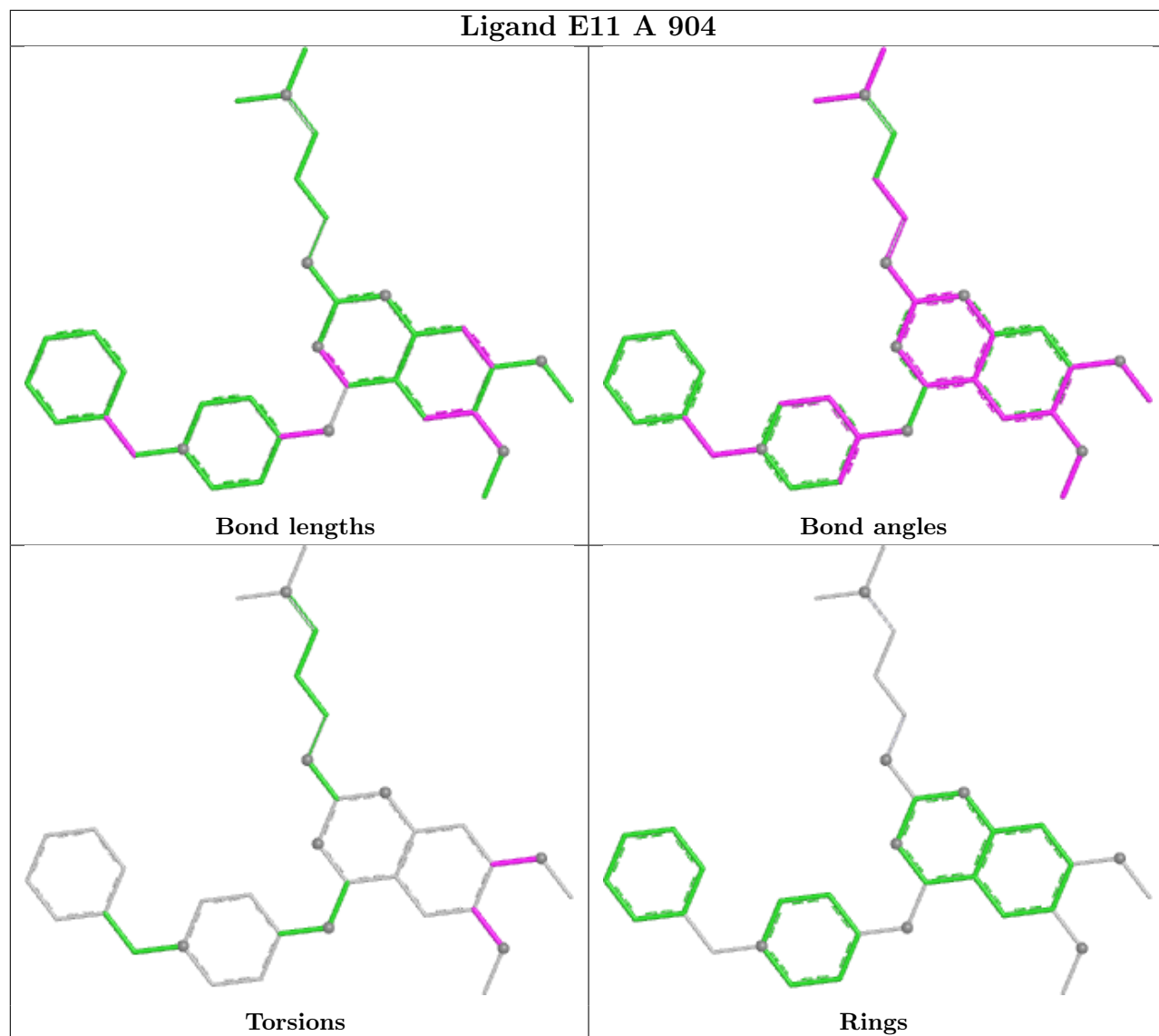


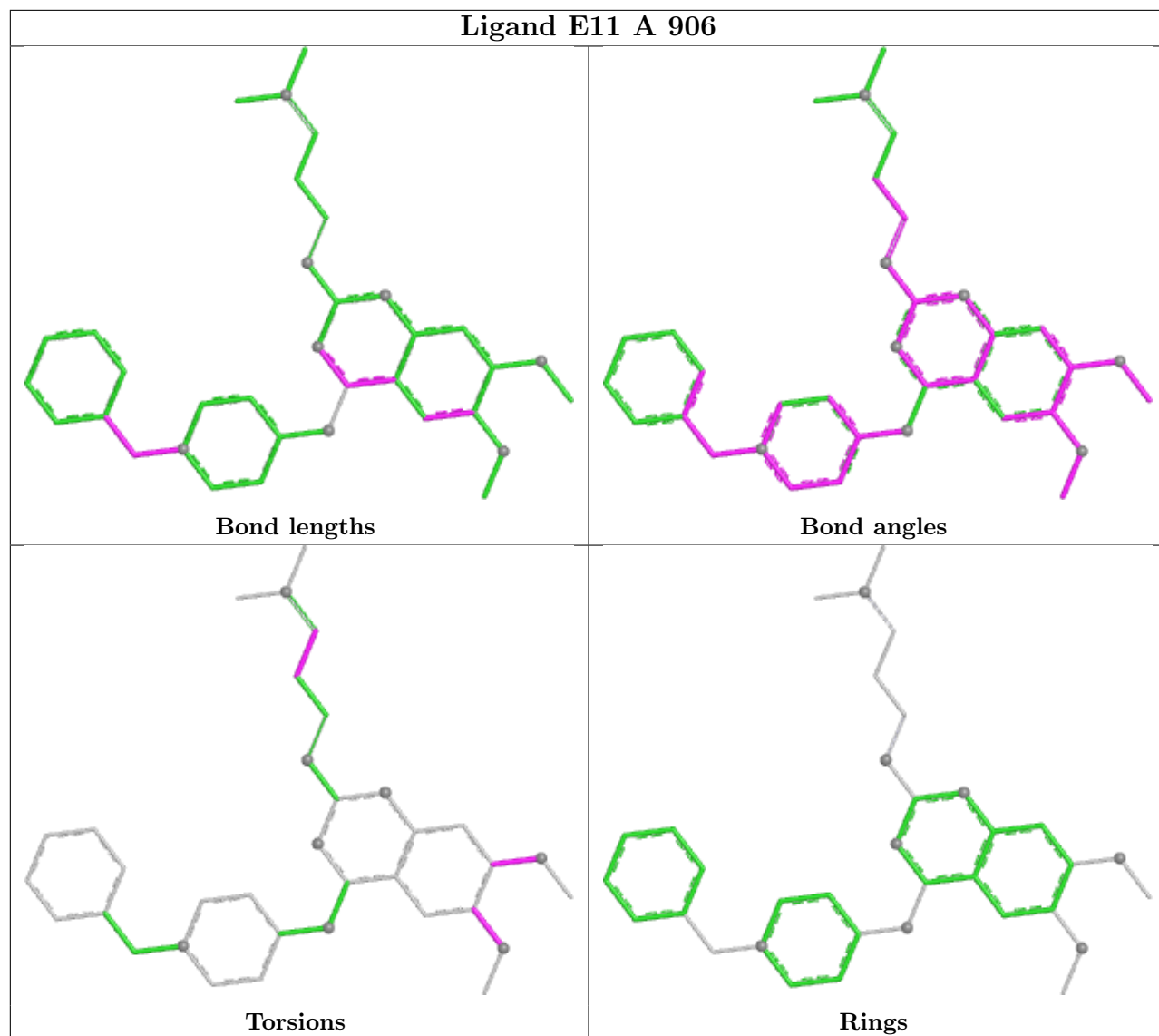
Ligand E11 A 902





Ligand E11 A 904





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	666/730 (91%)	0.14	33 (4%) 34 26	34, 64, 102, 130	0
2	B	133/178 (74%)	0.89	18 (13%) 7 5	58, 93, 127, 140	0
All	All	799/908 (87%)	0.27	51 (6%) 25 18	34, 69, 108, 140	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	ASN	5.6
1	A	836	LEU	5.5
1	A	171	PRO	5.4
2	B	340	MET	5.2
1	A	833	MET	4.7
2	B	376	ILE	4.6
1	A	275	THR	4.4
1	A	272	PRO	4.2
2	B	375	VAL	3.7
1	A	377	MET	3.7
2	B	308	ARG	3.5
1	A	699	LYS	3.4
2	B	385	THR	3.4
1	A	372	LYS	3.3
1	A	557	ASP	3.1
2	B	382	ARG	3.0
1	A	402	ASN	3.0
2	B	329	THR	2.9
2	B	361	GLU	2.7
1	A	273	LEU	2.7
2	B	312	LYS	2.7
1	A	350	ASN	2.7
1	A	517	SER	2.5
1	A	205	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	379	CYS	2.5
2	B	426	ARG	2.4
1	A	432	LYS	2.4
1	A	467	GLU	2.4
2	B	378	LYS	2.4
1	A	271	LYS	2.4
2	B	336	ARG	2.4
1	A	274	PRO	2.4
2	B	327	ASN	2.3
1	A	791	GLN	2.3
1	A	374	LYS	2.3
1	A	373	GLU	2.3
1	A	454	LYS	2.3
1	A	172	SER	2.3
1	A	645	GLU	2.2
1	A	771	ASN	2.2
1	A	358	GLN	2.2
2	B	309	LYS	2.2
1	A	268	LYS	2.1
1	A	568	ARG	2.1
2	B	440	GLU	2.1
1	A	792	PRO	2.1
2	B	332	THR	2.1
1	A	793	ILE	2.1
2	B	318	GLN	2.1
1	A	276	LYS	2.0
1	A	683	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

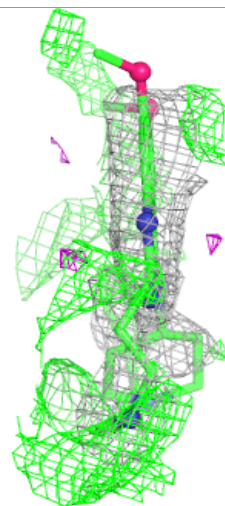
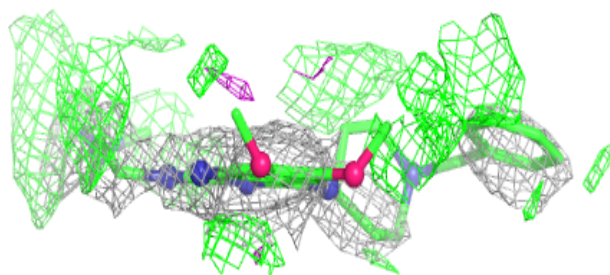
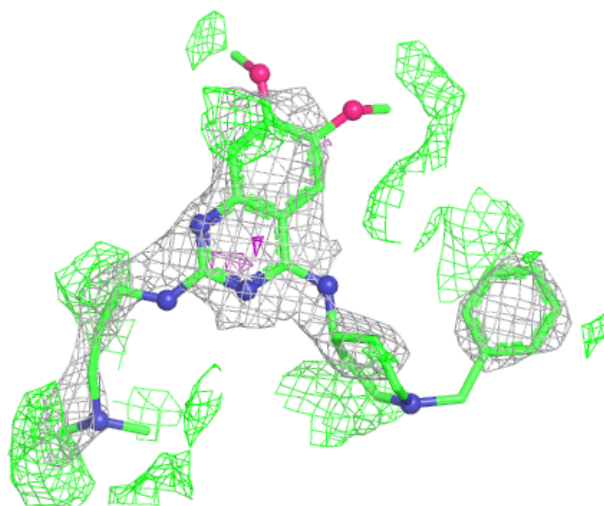
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	E11	A	906	35/35	0.75	0.49	125,153,172,177	0
4	E11	A	905	35/35	0.84	0.32	95,122,140,145	0
4	E11	A	904	35/35	0.85	0.31	74,103,154,164	0
4	E11	A	903	35/35	0.91	0.20	65,94,121,124	0
5	NA	A	907	1/1	0.93	0.21	55,55,55,55	0
4	E11	A	902	35/35	0.94	0.15	57,76,96,98	0
3	FAD	A	901	53/53	0.98	0.06	33,43,54,65	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.

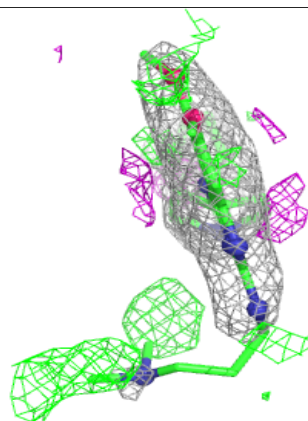
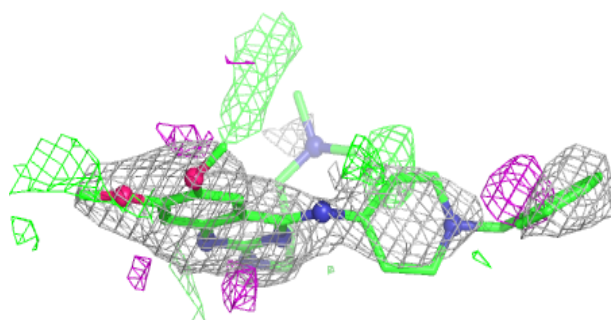
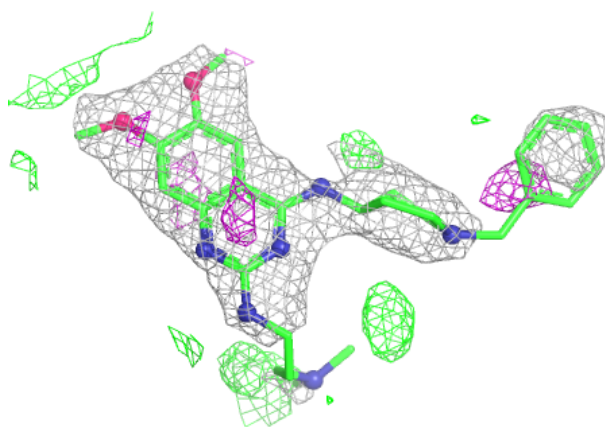
Electron density around E11 A 906:

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



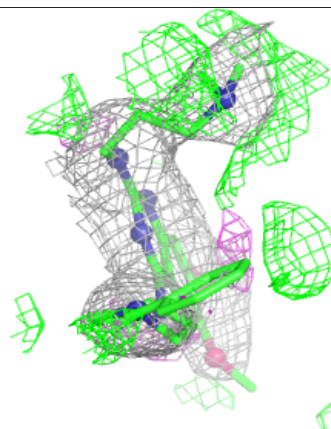
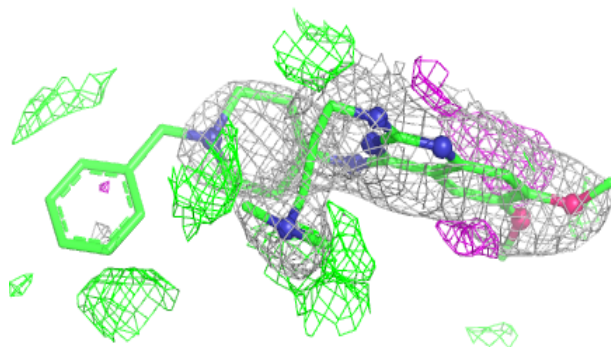
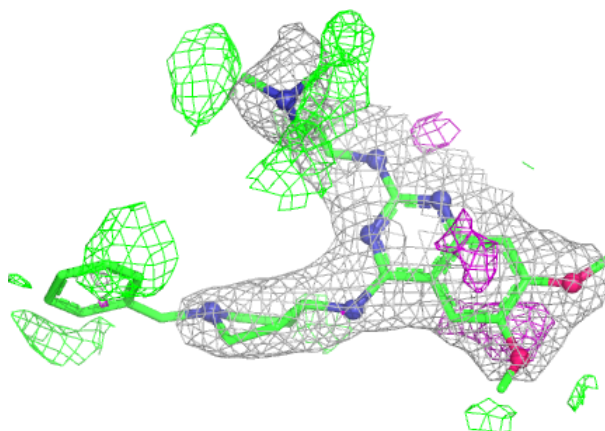
Electron density around E11 A 905:

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



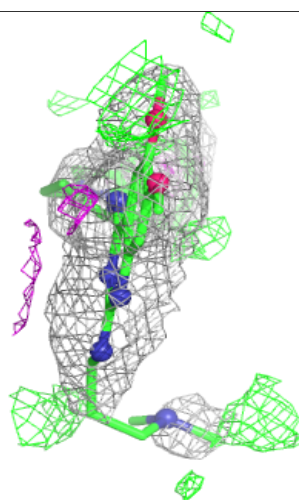
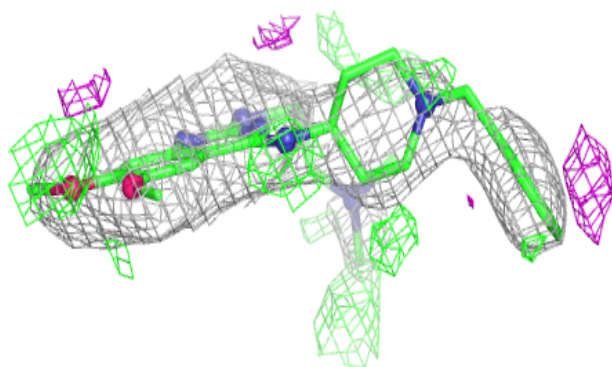
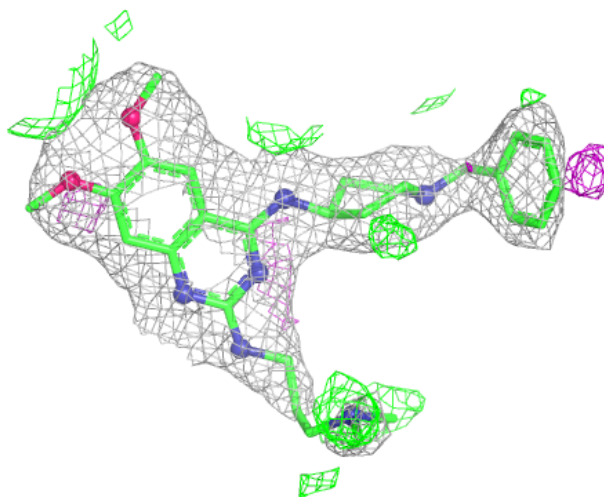
Electron density around E11 A 904:

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



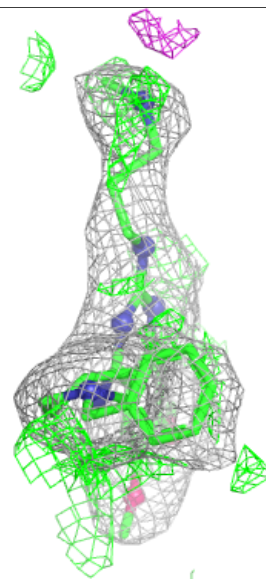
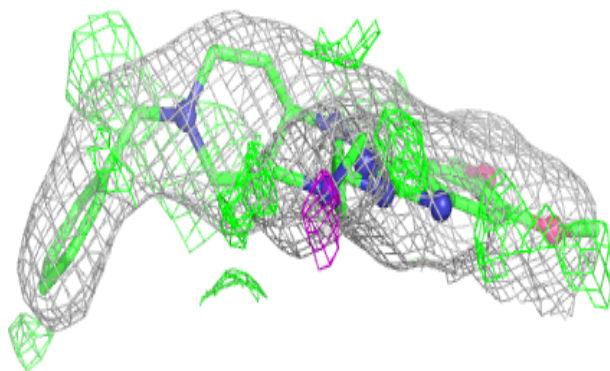
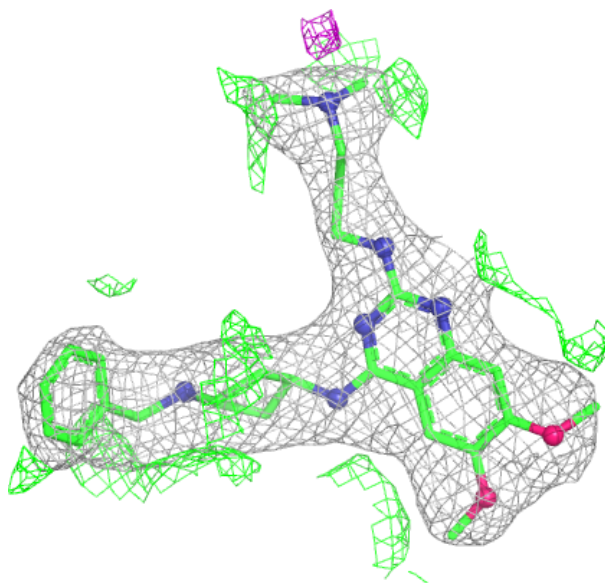
Electron density around E11 A 903:

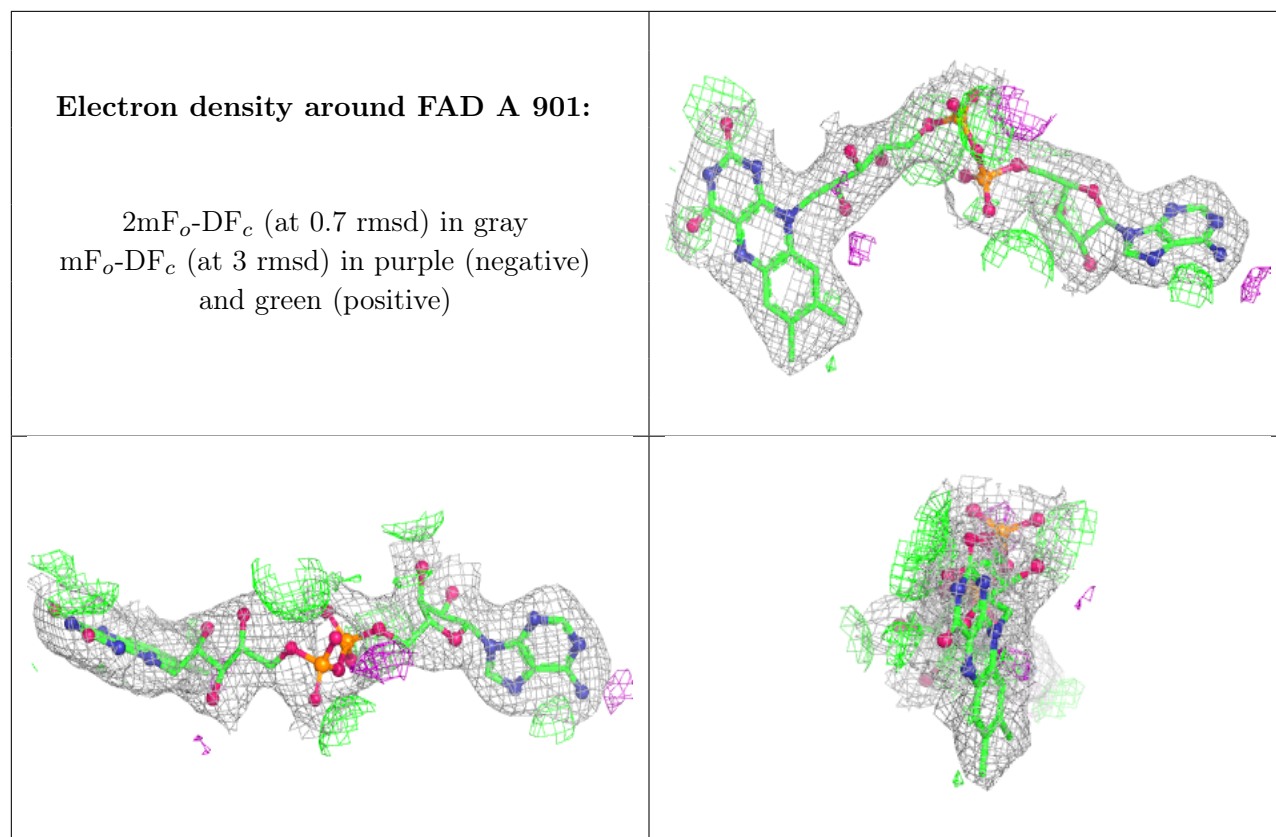
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around E11 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.