



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:42 PM UTC

PDB ID : 8P96 / pdb_00008p96
Title : TARGET COMPLEX 3
Authors : Garau, G.
Deposited on : 2023-06-05
Resolution : 2.86 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

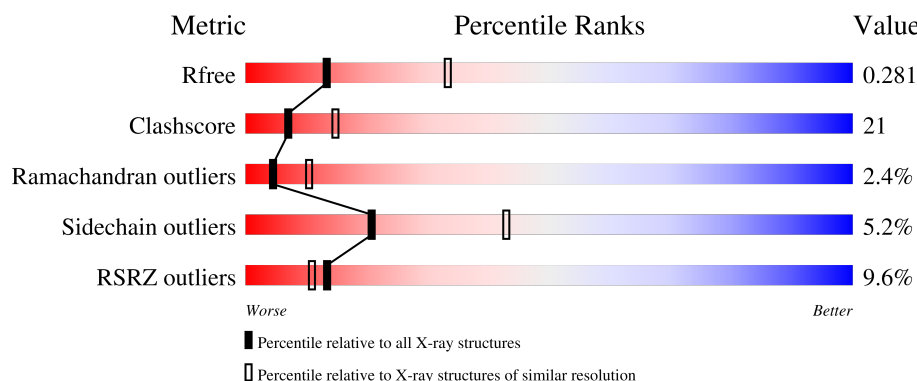
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	393	
1	B	393	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5946 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.

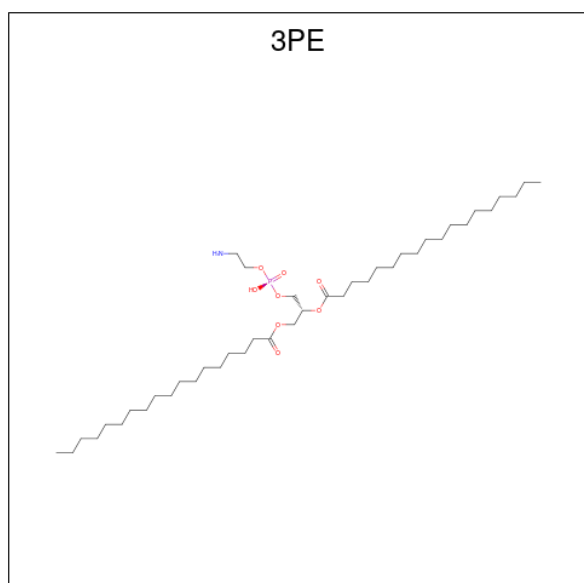
- Molecule 1 is a protein called N-acyl-phosphatidylethanolamine-hydrolyzing phospholipase D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	3	0
			2748	1778	467	489	14			
1	B	334	Total	C	N	O	S	0	3	0
			2754	1779	468	493	14			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

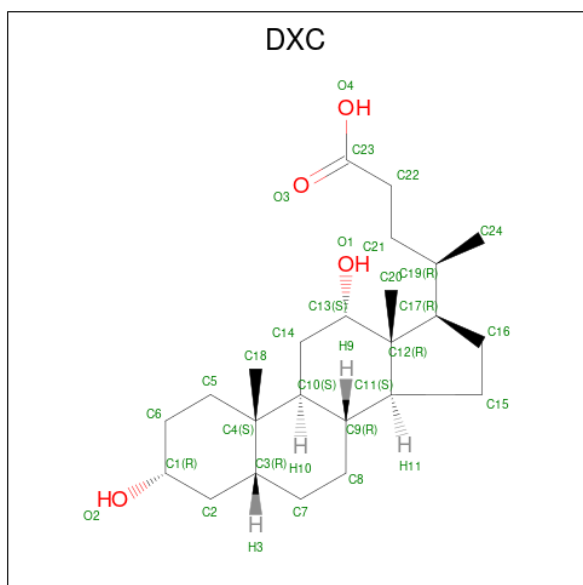
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

- Molecule 4 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (CCD ID: DXC) (formula: C₂₄H₄₀O₄) (labeled as "Ligand of Interest" by depositor).



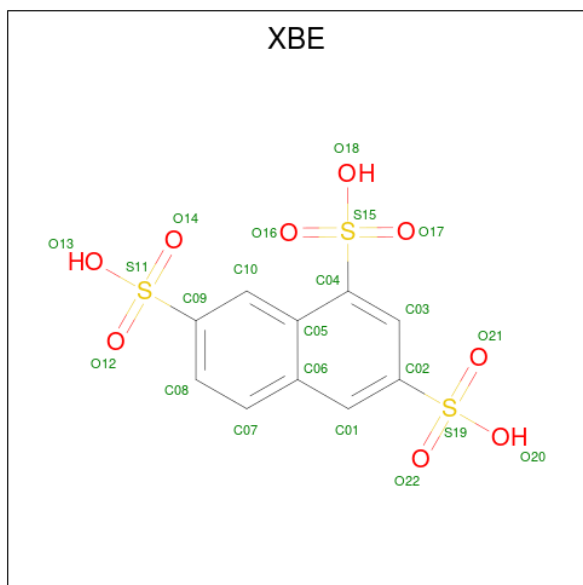
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			28	24	4		

- Molecule 5 is naphthalene-1,3,7-trisulfonic acid (CCD ID: XBE) (formula: $C_{10}H_8O_9S_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			22	10	9	3		

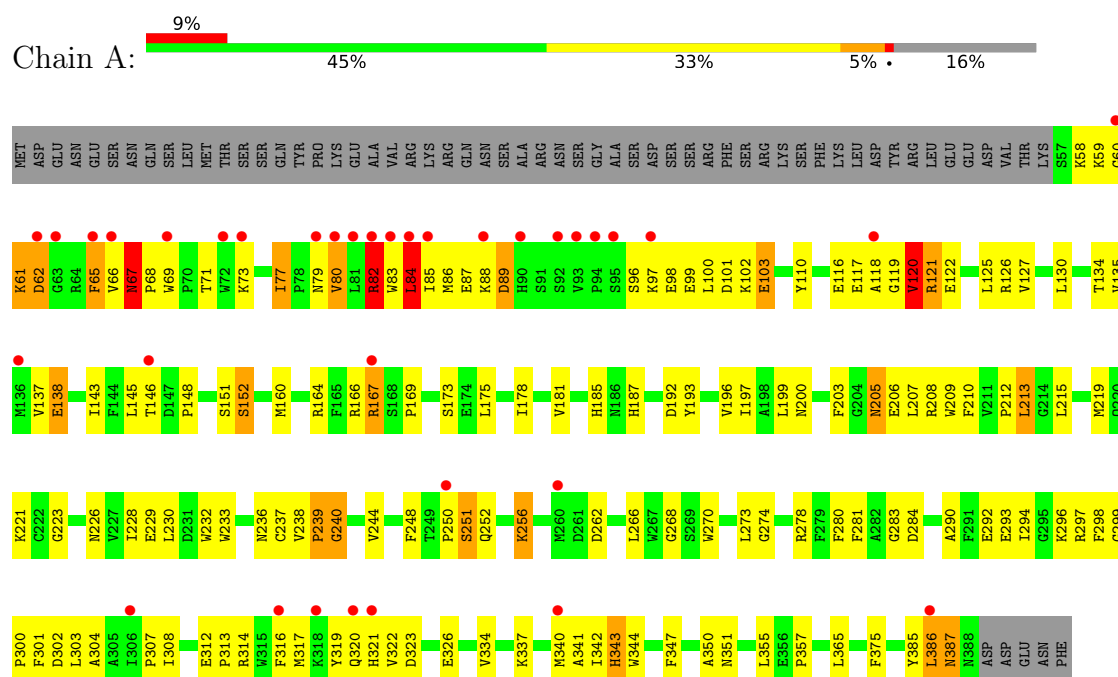
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		
6	B	30	Total	O	0	0
			30	30		

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: N-acyl-phosphatidylethanolamine-hydrolyzing phospholipase D



- Molecule 1: N-acyl-phosphatidylethanolamine-hydrolyzing phospholipase D





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	94.35Å 94.35Å 444.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.84 – 2.86 65.84 – 2.86	Depositor EDS
% Data completeness (in resolution range)	98.6 (65.84-2.86) 98.6 (65.84-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.253 , 0.281 0.253 , 0.281	Depositor DCC
R_{free} test set	1421 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5946	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: 3PE, XBE, DXC, ZN

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	0.36	0/2850	0.61	1/3880 (0.0%)
1	B	0.23	0/2856	0.55	0/3887
All	All	0.30	0/5706	0.58	1/7767 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	LEU	N-CA-C	-6.70	106.05	114.56

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	2748	0	2640	129	0
1	B	2754	0	2649	110	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	62	2	0
3	B	44	0	62	0	0
4	A	112	0	156	9	0
4	B	168	0	234	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	22	0	0	3	0
6	A	20	0	0	1	0
6	B	30	0	0	0	0
All	All	5946	0	5803	246	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 21.

All (246) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:HD23	1:B:139:MET:HB3	1.44	0.96
1:B:206:GLU:OE1	1:B:206:GLU:N	2.00	0.95
1:B:73:LYS:HG2	1:B:288:CYS:HB2	1.47	0.94
1:A:127:VAL:HG12	1:A:137:VAL:HG22	1.58	0.84
1:B:312:GLU:HB3	1:B:313:PRO:HD2	1.58	0.83
1:A:98:GLU:OE1	1:A:98:GLU:N	2.15	0.77
1:A:173:SER:HB2	1:B:97:LYS:HE2	1.70	0.73
4:A:405:DXC:H211	4:B:602:DXC:H81	1.70	0.73
1:B:235:GLU:HB3	1:B:247:VAL:HG22	1.72	0.72
1:A:103:GLU:HG3	1:A:355:LEU:HD11	1.72	0.72
1:B:273:LEU:HD12	1:B:278:ARG:HG2	1.73	0.71
1:A:135:VAL:HG21	1:A:340:MET:HE1	1.72	0.71
1:A:126:ARG:HB3	1:A:138:GLU:HG3	1.72	0.70
1:A:365:LEU:HD11	1:A:375:PHE:HB3	1.75	0.69
1:A:167[B]:ARG:NH1	5:B:610:XBE:O20	2.28	0.67
1:A:84:LEU:HD12	4:A:407:DXC:H142	1.77	0.67
1:A:213:LEU:HA	1:A:229:GLU:HG2	1.76	0.67
1:A:232:TRP:CE3	1:A:250:PRO:HA	2.30	0.66
1:A:97:LYS:HE3	1:B:202:ARG:HG3	1.77	0.66
1:B:312:GLU:CB	1:B:313:PRO:HD2	2.26	0.66
1:A:313:PRO:HD3	1:A:351:ASN:HD22	1.62	0.64
1:B:312:GLU:O	1:B:313:PRO:C	2.41	0.64
1:A:292:GLU:O	1:A:296:LYS:HG3	1.99	0.63
1:A:96:SER:O	1:A:99:GLU:N	2.31	0.63
1:A:69:TRP:CD1	1:A:266:LEU:HD13	2.34	0.62
1:A:85:ILE:HG22	1:A:85:ILE:O	2.00	0.62
1:A:120:VAL:HG22	1:A:138:GLU:HB2	1.80	0.62
1:A:303:LEU:HD21	1:A:386:LEU:HG	1.80	0.62
1:A:387:ASN:ND2	1:A:387:ASN:O	2.32	0.62
1:B:312:GLU:HG2	1:B:352:GLU:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASN:HB2	1:A:68:PRO:HD3	1.82	0.61
1:A:67:ASN:HD22	1:A:68:PRO:HD3	1.65	0.61
1:B:139:MET:HE1	1:B:279:PHE:HB3	1.82	0.61
1:A:151:SER:HA	5:B:610:XBE:O13	2.01	0.61
1:B:191:LEU:O	1:B:257:ARG:NH2	2.33	0.61
1:A:308:ILE:HD13	1:A:341:ALA:HB1	1.83	0.60
1:B:67:ASN:H	1:B:68:PRO:HD2	1.65	0.60
1:A:273:LEU:HD12	1:A:278:ARG:HG2	1.81	0.60
1:A:126:ARG:NH1	1:A:385:TYR:HB2	2.17	0.59
1:A:120:VAL:O	1:A:122:GLU:N	2.36	0.59
1:A:152:SER:HB2	1:A:167[B]:ARG:NH2	2.17	0.59
1:A:185:HIS:CD2	1:A:187:HIS:ND1	2.71	0.59
1:A:251:SER:HB3	1:A:268:GLY:HA2	1.83	0.59
1:B:73:LYS:HG3	1:B:289:PRO:HD2	1.83	0.59
1:B:72:TRP:CZ3	1:B:73:LYS:HD3	2.37	0.59
1:B:88:LYS:HE2	1:B:348:ALA:HB3	1.84	0.59
1:B:185:HIS:CD2	1:B:187:HIS:ND1	2.70	0.59
1:B:330:ILE:O	1:B:334:VAL:HG12	2.02	0.59
1:A:175:LEU:HD13	1:A:178:ILE:HD13	1.85	0.59
1:B:192:ASP:O	1:B:196:VAL:HG23	2.03	0.58
1:A:256:LYS:HG3	1:A:262:ASP:OD1	2.03	0.58
1:B:305:ALA:HB1	1:B:342:ILE:HG21	1.85	0.58
1:A:152:SER:HB2	1:A:167[B]:ARG:HH21	1.68	0.57
1:A:98:GLU:O	1:A:102:LYS:HD2	2.04	0.57
1:B:99:GLU:OE1	1:B:103:GLU:HG2	2.05	0.57
1:A:83:TRP:HE1	1:A:87:GLU:C	2.12	0.57
1:B:90:HIS:CD2	1:B:93:VAL:HG22	2.39	0.57
1:A:130:LEU:HA	1:A:169:PRO:HG2	1.86	0.57
1:A:290:ALA:O	1:A:294:ILE:HG13	2.04	0.57
1:B:136:MET:HE2	1:B:178:ILE:HD11	1.84	0.57
1:B:219:MET:HB3	1:B:227:VAL:HG11	1.85	0.56
1:B:365:LEU:HD11	1:B:375:PHE:HB3	1.85	0.56
1:A:79:ASN:HD21	1:A:319:TYR:HB2	1.70	0.56
1:B:65:PHE:O	1:B:66:VAL:C	2.48	0.56
1:B:314:ARG:NH1	1:B:326:GLU:OE1	2.38	0.55
1:A:205:ASN:C	1:A:207:LEU:H	2.15	0.55
1:B:134:THR:HG23	1:B:148:PRO:HA	1.88	0.55
1:B:217:ASP:O	1:B:221:LYS:HG2	2.07	0.55
1:A:316:PHE:CD2	1:A:317:MET:HE3	2.42	0.54
1:A:233:TRP:N	1:A:248:PHE:O	2.28	0.54
1:B:134:THR:HA	1:B:146:THR:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLY:N	1:B:229:GLU:OE2	2.37	0.54
1:B:200:ASN:ND2	1:B:223:GLY:O	2.40	0.54
1:B:232:TRP:CZ3	1:B:250:PRO:HA	2.42	0.54
1:B:86:MET:HE2	1:B:87:GLU:OE2	2.07	0.54
1:A:314:ARG:NH2	6:A:501:HOH:O	2.41	0.54
1:B:73:LYS:HB3	1:B:75:PRO:HD2	1.90	0.54
1:B:287:TYR:CE2	1:B:329:ARG:HB3	2.43	0.54
1:B:301:PHE:O	1:B:337:LYS:HG3	2.07	0.53
1:A:79:ASN:ND2	1:A:319:TYR:HB2	2.24	0.53
1:B:64:ARG:HA	1:B:69:TRP:HA	1.89	0.53
1:B:66:VAL:HG23	1:B:68:PRO:HD2	1.89	0.53
1:B:227:VAL:O	1:B:228:ILE:HD13	2.09	0.53
1:B:258:THR:HB	4:B:602:DXC:H1	1.91	0.53
1:B:218:TRP:HE3	1:B:219:MET:HE2	1.73	0.53
1:B:370:LEU:HD22	1:B:374:ASP:OD2	2.09	0.52
1:B:88:LYS:HG3	1:B:348:ALA:O	2.10	0.52
1:A:312:GLU:O	1:A:350:ALA:HB1	2.10	0.52
1:B:251:SER:HB3	1:B:268:GLY:HA2	1.91	0.52
1:A:121:ARG:O	1:A:122:GLU:C	2.52	0.52
1:B:308:ILE:HG12	1:B:341:ALA:HB1	1.92	0.52
1:A:207:LEU:HD23	1:A:209:TRP:CZ2	2.44	0.52
1:B:136:MET:HE1	1:B:176:PRO:HD2	1.91	0.52
1:B:139:MET:HE1	1:B:279:PHE:CB	2.40	0.52
1:A:61:LYS:HA	1:A:233:TRP:CD1	2.45	0.52
1:A:307:PRO:HA	1:A:342:ILE:O	2.10	0.52
1:A:116:GLU:C	1:A:118:ALA:H	2.18	0.51
1:A:120:VAL:HG12	1:A:121:ARG:H	1.73	0.51
1:B:90:HIS:CG	1:B:90:HIS:O	2.64	0.51
1:A:138:GLU:HB3	1:A:143:ILE:HG12	1.92	0.51
1:A:303:LEU:HD21	1:A:386:LEU:CG	2.39	0.51
1:A:145:LEU:HD13	1:A:148:PRO:HB3	1.91	0.51
1:A:387:ASN:C	1:A:387:ASN:HD22	2.11	0.51
1:B:175:LEU:O	1:B:202:ARG:NH1	2.41	0.51
1:B:64:ARG:HG3	1:B:68:PRO:O	2.10	0.51
4:A:406:DXC:H183	4:B:606:DXC:H203	1.93	0.50
1:B:72:TRP:CE3	1:B:73:LYS:HD3	2.47	0.50
1:B:285:THR:O	1:B:322:VAL:HG13	2.12	0.50
1:A:126:ARG:HB3	1:A:138:GLU:CG	2.42	0.50
1:A:196:VAL:HG13	1:A:209:TRP:CH2	2.47	0.50
1:A:67:ASN:ND2	1:A:68:PRO:HD3	2.27	0.49
1:A:207:LEU:O	1:A:226:ASN:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:THR:C	1:A:73:LYS:H	2.21	0.49
1:A:87:GLU:HB3	1:A:351:ASN:HD21	1.77	0.49
1:A:278:ARG:HH11	1:A:278:ARG:HB2	1.77	0.49
1:B:172:ILE:HD12	1:B:199:LEU:HD22	1.94	0.49
1:A:77:ILE:HG12	1:A:319:TYR:CD2	2.46	0.49
1:B:67:ASN:H	1:B:68:PRO:CD	2.24	0.49
1:A:67:ASN:CB	1:A:68:PRO:HD3	2.42	0.49
3:A:403:3PE:H2A1	3:A:403:3PE:H3D2	1.95	0.49
1:A:314:ARG:NH1	1:A:323:ASP:OD2	2.46	0.49
1:B:218:TRP:NE1	4:B:607:DXC:H3	2.27	0.48
1:B:229:GLU:O	1:B:230:LEU:HD23	2.12	0.48
1:A:88:LYS:O	1:A:89:ASP:C	2.56	0.48
1:B:311:TYR:OH	1:B:360:LYS:HD2	2.13	0.48
1:A:122:GLU:HB3	1:A:385:TYR:OH	2.14	0.48
1:B:62:ASP:OD1	1:B:62:ASP:N	2.40	0.47
1:B:142:LEU:CD1	1:B:244:VAL:HG11	2.43	0.47
1:B:151:SER:OG	5:B:610:XBE:O17	2.24	0.47
1:A:62:ASP:OD2	1:A:232:TRP:HZ2	1.97	0.47
1:A:67:ASN:HD22	1:A:68:PRO:CD	2.27	0.47
1:A:80:VAL:O	1:A:316:PHE:HZ	1.97	0.47
1:A:110:TYR:OH	1:A:138:GLU:OE2	2.25	0.47
1:B:82:ARG:HE	1:B:256:LYS:HE2	1.78	0.47
1:B:69:TRP:CD1	1:B:69:TRP:N	2.83	0.47
1:A:290:ALA:HA	1:A:293:GLU:HB2	1.96	0.47
1:A:65:PHE:C	1:A:67:ASN:N	2.72	0.47
1:A:192:ASP:O	1:A:196:VAL:HG23	2.15	0.47
1:A:236:ASN:OD1	1:A:237:CYS:N	2.37	0.47
1:A:387:ASN:ND2	1:A:387:ASN:C	2.68	0.47
1:B:209:TRP:HB2	1:B:227:VAL:HG12	1.97	0.47
1:A:118:ALA:O	1:A:120:VAL:HG23	2.15	0.47
1:B:62:ASP:HA	1:B:63:GLY:HA3	1.65	0.47
1:A:208:ARG:NH1	1:A:228:ILE:HD11	2.30	0.46
1:A:343:HIS:O	1:A:344:TRP:CD1	2.68	0.46
1:A:71:THR:HG21	1:A:252:GLN:HG2	1.97	0.46
1:A:145:LEU:O	1:A:181:VAL:HA	2.15	0.46
1:A:185:HIS:CE1	1:A:284:ASP:HB2	2.51	0.46
1:B:315:TRP:CZ3	1:B:316:PHE:HB2	2.51	0.46
1:B:140:ASP:OD2	1:B:275:PRO:HD2	2.16	0.46
1:B:326:GLU:HA	1:B:329:ARG:HB2	1.97	0.46
1:B:258:THR:HG21	4:B:602:DXC:H3	1.97	0.46
1:A:210:PHE:HB3	1:A:270:TRP:CH2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:HD13	1:B:148:PRO:HB3	1.98	0.45
1:B:185:HIS:CE1	1:B:284:ASP:HB2	2.51	0.45
1:A:60:GLY:C	1:A:233:TRP:HE1	2.24	0.45
1:B:109:PRO:HG2	1:B:170:CYS:HB3	1.98	0.45
1:A:85:ILE:O	1:A:85:ILE:CG2	2.63	0.45
1:B:216:LEU:HB2	1:B:229:GLU:CD	2.42	0.45
1:B:208:ARG:NH1	1:B:237:CYS:O	2.50	0.45
1:A:164:ARG:HB3	1:A:347:PHE:CE1	2.52	0.44
1:A:193:TYR:HE2	1:B:159:TYR:HA	1.82	0.44
4:A:407:DXC:H243	4:A:407:DXC:H221	1.77	0.44
1:B:139:MET:O	1:B:139:MET:HG3	2.17	0.44
1:B:353:HIS:HB3	1:B:356:GLU:HB2	1.98	0.44
1:A:58:LYS:O	1:A:59:LYS:C	2.60	0.44
1:B:218:TRP:CE3	1:B:219:MET:HE2	2.51	0.44
1:B:312:GLU:O	1:B:314:ARG:N	2.51	0.44
1:A:100:LEU:HB3	1:A:166:ARG:NH2	2.33	0.44
1:B:292:GLU:O	1:B:296:LYS:HG3	2.17	0.44
1:B:305:ALA:HB1	1:B:342:ILE:HD13	2.00	0.44
1:B:311:TYR:CD1	1:B:311:TYR:O	2.70	0.44
1:A:278:ARG:NH1	1:A:300:PRO:O	2.50	0.44
1:A:297:ARG:HG3	1:A:298:PHE:CE1	2.52	0.44
1:B:65:PHE:H	1:B:70:PRO:HD3	1.83	0.44
1:A:83:TRP:CZ2	1:A:88:LYS:HA	2.52	0.43
1:A:302:ASP:OD1	1:A:337:LYS:HE3	2.18	0.43
1:A:322:VAL:HB	1:A:326:GLU:HB2	2.00	0.43
1:B:99:GLU:OE1	1:B:99:GLU:O	2.35	0.43
1:B:314:ARG:O	1:B:315:TRP:C	2.60	0.43
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.83	0.43
1:B:191:LEU:HD11	1:B:219:MET:HE1	2.01	0.43
1:B:203:PHE:HB2	1:B:207:LEU:HD22	2.00	0.43
1:A:87:GLU:O	1:A:88:LYS:C	2.61	0.43
1:A:167[A]:ARG:HH21	1:A:169:PRO:HA	1.83	0.43
1:A:308:ILE:O	1:A:357:PRO:HB3	2.19	0.43
1:A:82:ARG:H	1:A:82:ARG:NH1	2.17	0.43
1:A:215:LEU:O	1:A:219:MET:HG2	2.18	0.43
1:A:239:PRO:O	1:A:240:GLY:C	2.60	0.43
1:B:145:LEU:HD23	1:B:145:LEU:HA	1.93	0.43
1:A:130:LEU:HD12	1:A:134:THR:HG22	2.00	0.43
1:B:65:PHE:H	1:B:70:PRO:CD	2.32	0.43
1:B:216:LEU:HB2	1:B:229:GLU:HG3	2.01	0.43
1:A:83:TRP:CE2	1:A:88:LYS:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:SER:O	1:A:97:LYS:C	2.62	0.43
1:A:125:LEU:O	1:A:386:LEU:N	2.52	0.43
3:A:403:3PE:H2B1	4:B:601:DXC:H1	1.99	0.43
1:B:343:HIS:O	1:B:344:TRP:CD1	2.71	0.43
1:A:71:THR:HG21	1:A:252:GLN:CG	2.49	0.42
1:A:208:ARG:HG2	1:A:238:VAL:HG12	2.01	0.42
1:B:67:ASN:N	1:B:68:PRO:CD	2.82	0.42
1:A:61:LYS:HA	1:A:233:TRP:HD1	1.83	0.42
1:A:117:GLU:C	1:A:119:GLY:N	2.75	0.42
1:A:134:THR:HA	1:A:146:THR:O	2.19	0.42
4:A:406:DXC:C18	4:B:606:DXC:H203	2.49	0.42
1:B:233:TRP:N	1:B:248:PHE:O	2.50	0.42
1:B:88:LYS:O	1:B:89:ASP:C	2.63	0.42
1:B:175:LEU:HD13	1:B:178:ILE:HG12	2.01	0.42
1:A:299:GLY:HA2	1:A:300:PRO:C	2.43	0.42
1:A:213:LEU:HD23	1:A:230:LEU:C	2.45	0.42
4:A:405:DXC:H211	4:B:602:DXC:H151	2.02	0.42
1:B:310:ALA:N	1:B:352:GLU:OE2	2.46	0.42
1:A:65:PHE:O	1:A:67:ASN:N	2.53	0.42
1:A:199:LEU:O	1:A:203:PHE:N	2.53	0.42
1:A:317:MET:HE2	1:A:317:MET:HA	2.02	0.42
1:B:280:PHE:O	1:B:304:ALA:HA	2.19	0.42
1:A:281:PHE:CZ	1:A:283:GLY:HA2	2.55	0.41
4:A:405:DXC:H3	4:A:407:DXC:C20	2.50	0.41
1:B:130:LEU:HA	1:B:169:PRO:HG2	2.01	0.41
1:B:213:LEU:HD13	1:B:230:LEU:C	2.45	0.41
1:B:296:LYS:HE3	1:B:296:LYS:HB3	1.90	0.41
1:B:73:LYS:CG	1:B:289:PRO:HD2	2.51	0.41
1:B:120:VAL:HG13	1:B:122:GLU:N	2.35	0.41
1:B:196:VAL:HG13	1:B:209:TRP:CH2	2.55	0.41
1:B:251:SER:OG	1:B:285:THR:HB	2.20	0.41
1:A:96:SER:C	1:A:98:GLU:OE1	2.64	0.41
1:A:200:ASN:ND2	1:A:223:GLY:O	2.51	0.41
1:A:280:PHE:O	1:A:304:ALA:HA	2.20	0.41
1:A:301:PHE:CE1	1:A:334:VAL:HG22	2.54	0.41
4:A:405:DXC:H161	4:A:405:DXC:H212	1.70	0.41
1:A:244:VAL:HG23	1:A:274:GLY:HA2	2.01	0.41
1:A:160:MET:HE2	1:A:160:MET:HB3	1.75	0.41
1:A:193:TYR:CE1	1:A:197:ILE:HD11	2.55	0.41
1:B:259:LEU:CD2	4:B:609:DXC:H72	2.50	0.41
1:A:208:ARG:HD2	1:A:208:ARG:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:405:DXC:C21	4:B:602:DXC:H151	2.51	0.41
1:A:212:PRO:HB3	1:A:266:LEU:HB3	2.03	0.41
1:A:134:THR:HG23	1:A:148:PRO:HA	2.03	0.41
1:A:221:LYS:HB3	1:A:221:LYS:HE3	1.60	0.41
1:B:59:LYS:HD2	1:B:233:TRP:CG	2.56	0.41
1:A:117:GLU:O	1:A:119:GLY:N	2.55	0.40
1:A:135:VAL:HG13	1:A:146:THR:HB	2.03	0.40
1:A:320:GLN:O	1:A:321:HIS:HD2	2.04	0.40
1:B:262:ASP:OD1	1:B:262:ASP:N	2.54	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	333/393 (85%)	283 (85%)	39 (12%)	11 (3%)	3	7
1	B	335/393 (85%)	291 (87%)	39 (12%)	5 (2%)	8	18
All	All	668/786 (85%)	574 (86%)	78 (12%)	16 (2%)	4	10

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	VAL
1	B	66	VAL
1	B	313	PRO
1	A	67	ASN
1	B	312	GLU
1	A	61	LYS
1	A	82	ARG
1	A	86	MET
1	A	121	ARG

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Mol	Chain	Res	Type
1	A	240	GLY
1	A	66	VAL
1	A	89	ASP
1	A	206	GLU
1	A	239	PRO
1	B	344	TRP
1	B	67	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/352 (85%)	277 (93%)	21 (7%)	14	29
1	B	299/352 (85%)	288 (96%)	11 (4%)	30	55
All	All	597/704 (85%)	565 (95%)	32 (5%)	21	42

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

Mol	Chain	Res	Type
1	A	62	ASP
1	A	65	PHE
1	A	67	ASN
1	A	77	ILE
1	A	80	VAL
1	A	82	ARG
1	A	84	LEU
1	A	101	ASP
1	A	103	GLU
1	A	120	VAL
1	A	138	GLU
1	A	152	SER
1	A	167[A]	ARG
1	A	167[B]	ARG
1	A	205	ASN
1	A	213	LEU

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Mol	Chain	Res	Type
1	A	251	SER
1	A	256	LYS
1	A	343	HIS
1	A	386	LEU
1	A	387	ASN
1	B	66	VAL
1	B	67	ASN
1	B	85	ILE
1	B	125	LEU
1	B	155	SER
1	B	242	ASP
1	B	312	GLU
1	B	313	PRO
1	B	314	ARG
1	B	343	HIS
1	B	377	VAL

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	67	ASN
1	A	79	ASN
1	A	252	GLN
1	A	263	ASN
1	A	277	ASN
1	A	351	ASN
1	A	387	ASN
1	B	90	HIS
1	B	252	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	DXC	B	609	-	31,31,31	0.60	0	49,49,49	0.98	2 (4%)
4	DXC	A	405	-	31,31,31	0.63	0	49,49,49	0.89	0
4	DXC	A	407	-	31,31,31	0.59	0	49,49,49	0.94	0
4	DXC	B	608	-	31,31,31	0.62	0	49,49,49	1.01	3 (6%)
5	XBE	B	610	-	22,23,23	1.40	3 (13%)	36,38,38	1.26	7 (19%)
4	DXC	B	606	-	31,31,31	0.61	0	49,49,49	1.00	2 (4%)
4	DXC	B	607	-	31,31,31	0.57	0	49,49,49	0.86	1 (2%)
4	DXC	B	601	-	31,31,31	0.58	0	49,49,49	0.86	1 (2%)
3	3PE	B	605	2	43,43,50	0.54	0	46,48,55	0.63	1 (2%)
4	DXC	A	404	-	31,31,31	0.58	0	49,49,49	0.79	0
4	DXC	A	406	-	31,31,31	0.67	0	49,49,49	1.14	2 (4%)
4	DXC	B	602	-	31,31,31	0.69	0	49,49,49	1.50	7 (14%)
3	3PE	A	403	2	43,43,50	0.55	0	46,48,55	0.70	2 (4%)

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	DXC	B	609	-	-	5/9/71/71	0/4/4/4
4	DXC	A	405	-	-	5/9/71/71	0/4/4/4
4	DXC	A	407	-	-	8/9/71/71	0/4/4/4
4	DXC	B	608	-	-	3/9/71/71	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	XBE	B	610	-	-	6/18/18/18	0/2/2/2
4	DXC	B	606	-	-	0/9/71/71	0/4/4/4
4	DXC	B	607	-	-	7/9/71/71	0/4/4/4
4	DXC	B	601	-	-	0/9/71/71	0/4/4/4
3	3PE	B	605	2	-	22/47/47/54	-
4	DXC	A	404	-	-	5/9/71/71	0/4/4/4
4	DXC	A	406	-	-	9/9/71/71	0/4/4/4
4	DXC	B	602	-	-	4/9/71/71	0/4/4/4
3	3PE	A	403	2	-	18/47/47/54	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	610	XBE	C05-C06	-2.70	1.38	1.43
5	B	610	XBE	C09-S11	2.39	1.82	1.77
5	B	610	XBE	C02-S19	2.19	1.81	1.77

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	406	DXC	C11-C9-C10	-3.73	104.22	109.09
4	B	602	DXC	C14-C13-C12	3.55	114.87	111.26
4	B	602	DXC	C15-C11-C12	3.46	106.90	103.54
4	B	602	DXC	C11-C9-C10	-3.32	104.74	109.09
4	B	602	DXC	C12-C11-C9	-3.32	111.12	114.69
4	A	406	DXC	C16-C15-C11	-3.29	98.70	105.14
4	B	602	DXC	C8-C9-C10	3.28	114.45	110.52
4	B	602	DXC	C10-C14-C13	3.13	118.39	114.29
5	B	610	XBE	O16-S15-C04	2.90	114.77	106.37
4	B	606	DXC	C12-C11-C9	-2.60	111.89	114.69
3	A	403	3PE	C2-O21-C21	2.51	123.80	117.80
3	B	605	3PE	O12-P-O14	2.47	123.95	112.44
5	B	610	XBE	O17-S15-O16	-2.45	100.54	112.88
4	B	606	DXC	C17-C12-C11	2.40	102.52	100.11
3	A	403	3PE	O12-P-O14	2.37	123.46	112.44
4	B	609	DXC	C16-C15-C11	-2.34	100.56	105.14
5	B	610	XBE	O14-S11-C09	2.27	111.89	106.68
4	B	608	DXC	C12-C17-C19	2.24	122.20	119.48
5	B	610	XBE	O22-S19-O21	-2.23	101.65	112.88
5	B	610	XBE	O14-S11-O12	-2.14	102.11	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	610	XBE	C04-C05-C06	2.14	119.99	117.40
4	B	608	DXC	C11-C9-C10	-2.12	106.32	109.09
4	B	607	DXC	C16-C17-C12	-2.11	101.49	103.54
4	B	602	DXC	C17-C12-C13	2.08	119.53	117.67
4	B	609	DXC	C15-C11-C12	-2.07	101.54	103.54
5	B	610	XBE	O22-S19-C02	2.02	111.31	106.68
4	B	608	DXC	C8-C9-C10	2.02	112.93	110.52
4	B	601	DXC	C24-C19-C17	2.01	115.91	112.88

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	3PE	C1-O11-P-O13
3	A	403	3PE	C1-O11-P-O14
3	A	403	3PE	O13-C11-C12-N
3	B	605	3PE	C1-O11-P-O12
3	B	605	3PE	C1-O11-P-O13
3	B	605	3PE	C1-O11-P-O14
3	B	605	3PE	C11-O13-P-O12
3	B	605	3PE	C11-O13-P-O14
3	B	605	3PE	O13-C11-C12-N
5	B	610	XBE	C03-C04-S15-O16
5	B	610	XBE	C03-C04-S15-O18
5	B	610	XBE	C05-C04-S15-O17
5	B	610	XBE	C05-C04-S15-O18
4	B	609	DXC	C24-C19-C21-C22
3	A	403	3PE	C32-C31-O31-C3
3	B	605	3PE	C32-C31-O31-C3
3	A	403	3PE	O32-C31-O31-C3
3	B	605	3PE	O32-C31-O31-C3
4	B	608	DXC	C24-C19-C21-C22
4	A	405	DXC	C17-C19-C21-C22
4	A	406	DXC	C17-C19-C21-C22
4	A	406	DXC	C19-C21-C22-C23
4	A	406	DXC	C24-C19-C21-C22
4	A	404	DXC	C24-C19-C21-C22
4	A	406	DXC	C12-C17-C19-C21
4	A	406	DXC	C16-C17-C19-C24
4	B	607	DXC	C24-C19-C21-C22
3	A	403	3PE	C29-C2A-C2B-C2C
3	B	605	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
3	A	403	3PE	C21-C22-C23-C24
4	A	406	DXC	C12-C17-C19-C24
3	B	605	3PE	C26-C27-C28-C29
5	B	610	XBE	C05-C04-S15-O16
4	B	602	DXC	C19-C21-C22-C23
4	A	406	DXC	C16-C17-C19-C21
3	B	605	3PE	C25-C26-C27-C28
3	B	605	3PE	C21-C22-C23-C24
5	B	610	XBE	C03-C04-S15-O17
4	A	407	DXC	C19-C21-C22-C23
3	B	605	3PE	C2A-C2B-C2C-C2D
3	A	403	3PE	C27-C28-C29-C2A
4	B	607	DXC	C12-C17-C19-C24
3	A	403	3PE	C2A-C2B-C2C-C2D
3	A	403	3PE	C3A-C3B-C3C-C3D
3	B	605	3PE	C3A-C3B-C3C-C3D
4	A	407	DXC	C12-C17-C19-C24
4	A	407	DXC	C12-C17-C19-C21
4	B	607	DXC	C12-C17-C19-C21
3	A	403	3PE	C2B-C2C-C2D-C2E
3	B	605	3PE	C2B-C2C-C2D-C2E
3	B	605	3PE	C27-C28-C29-C2A
3	B	605	3PE	C39-C3A-C3B-C3C
4	B	607	DXC	C16-C17-C19-C24
3	A	403	3PE	C23-C24-C25-C26
3	A	403	3PE	C39-C3A-C3B-C3C
3	B	605	3PE	C23-C24-C25-C26
4	A	407	DXC	C16-C17-C19-C21
4	A	407	DXC	C16-C17-C19-C24
4	B	607	DXC	C16-C17-C19-C21
4	B	609	DXC	C17-C19-C21-C22
3	A	403	3PE	C11-O13-P-O11
3	A	403	3PE	C11-O13-P-O12
3	A	403	3PE	C11-O13-P-O14
3	B	605	3PE	C11-O13-P-O11
4	A	404	DXC	C12-C17-C19-C24
3	A	403	3PE	C31-C32-C33-C34
3	B	605	3PE	C31-C32-C33-C34
4	A	404	DXC	C12-C17-C19-C21
3	B	605	3PE	C32-C33-C34-C35
4	A	407	DXC	C21-C22-C23-O3
3	A	403	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
4	B	609	DXC	C21-C22-C23-O3
4	A	407	DXC	C21-C22-C23-O4
4	A	405	DXC	C24-C19-C21-C22
4	B	607	DXC	C21-C22-C23-O4
4	A	406	DXC	C21-C22-C23-O3
4	B	607	DXC	C21-C22-C23-O3
4	A	406	DXC	C21-C22-C23-O4
4	A	407	DXC	C24-C19-C21-C22
4	B	602	DXC	C16-C17-C19-C21
4	B	609	DXC	C21-C22-C23-O4
4	B	602	DXC	C12-C17-C19-C21
4	A	405	DXC	C21-C22-C23-O4
4	A	404	DXC	C16-C17-C19-C21
4	B	608	DXC	C21-C22-C23-O4
3	B	605	3PE	O11-C1-C2-O21
4	B	609	DXC	C19-C21-C22-C23
4	A	405	DXC	C21-C22-C23-O3
4	A	405	DXC	C16-C17-C19-C21
4	B	608	DXC	C21-C22-C23-O3
4	B	602	DXC	C12-C17-C19-C24
4	A	404	DXC	C21-C22-C23-O3

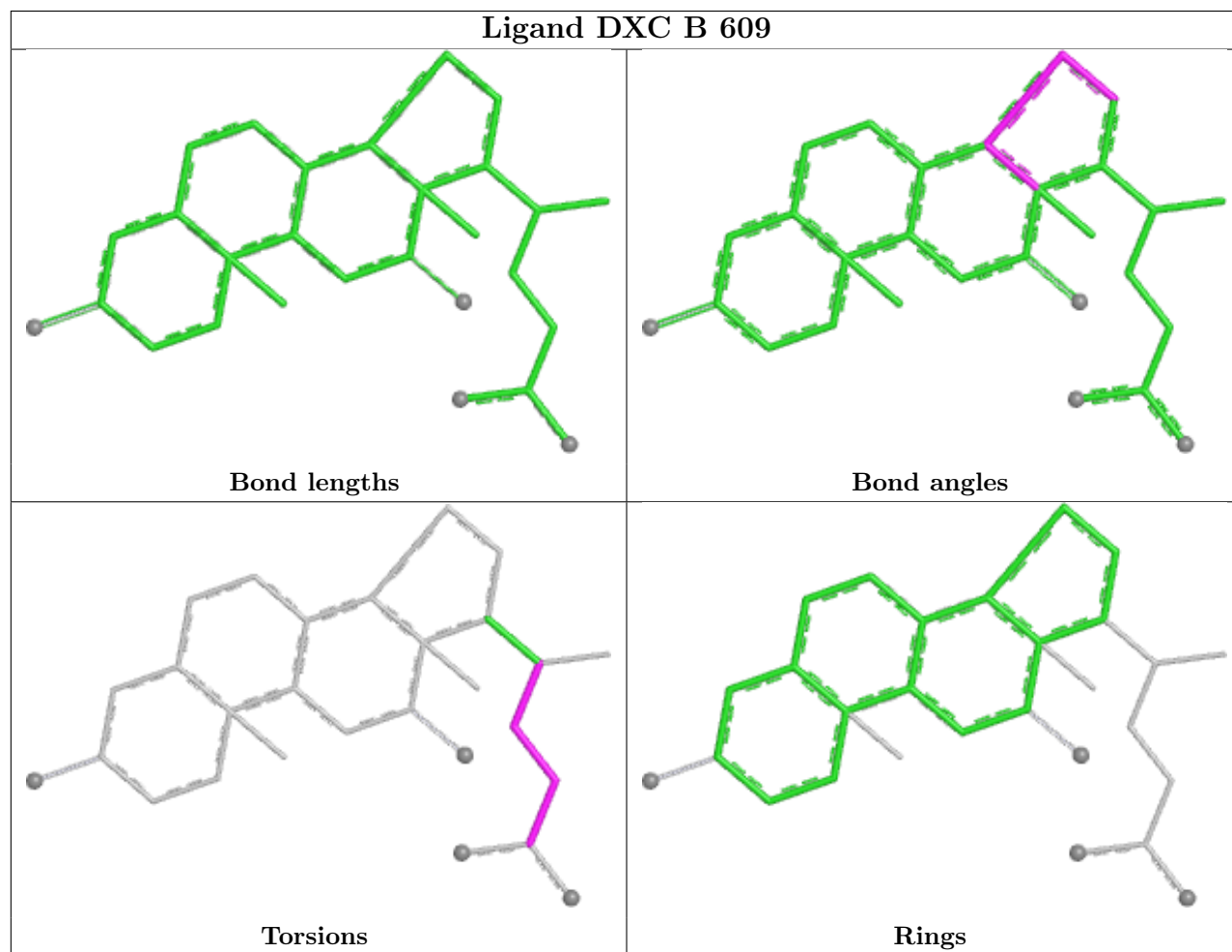
There are no ring outliers.

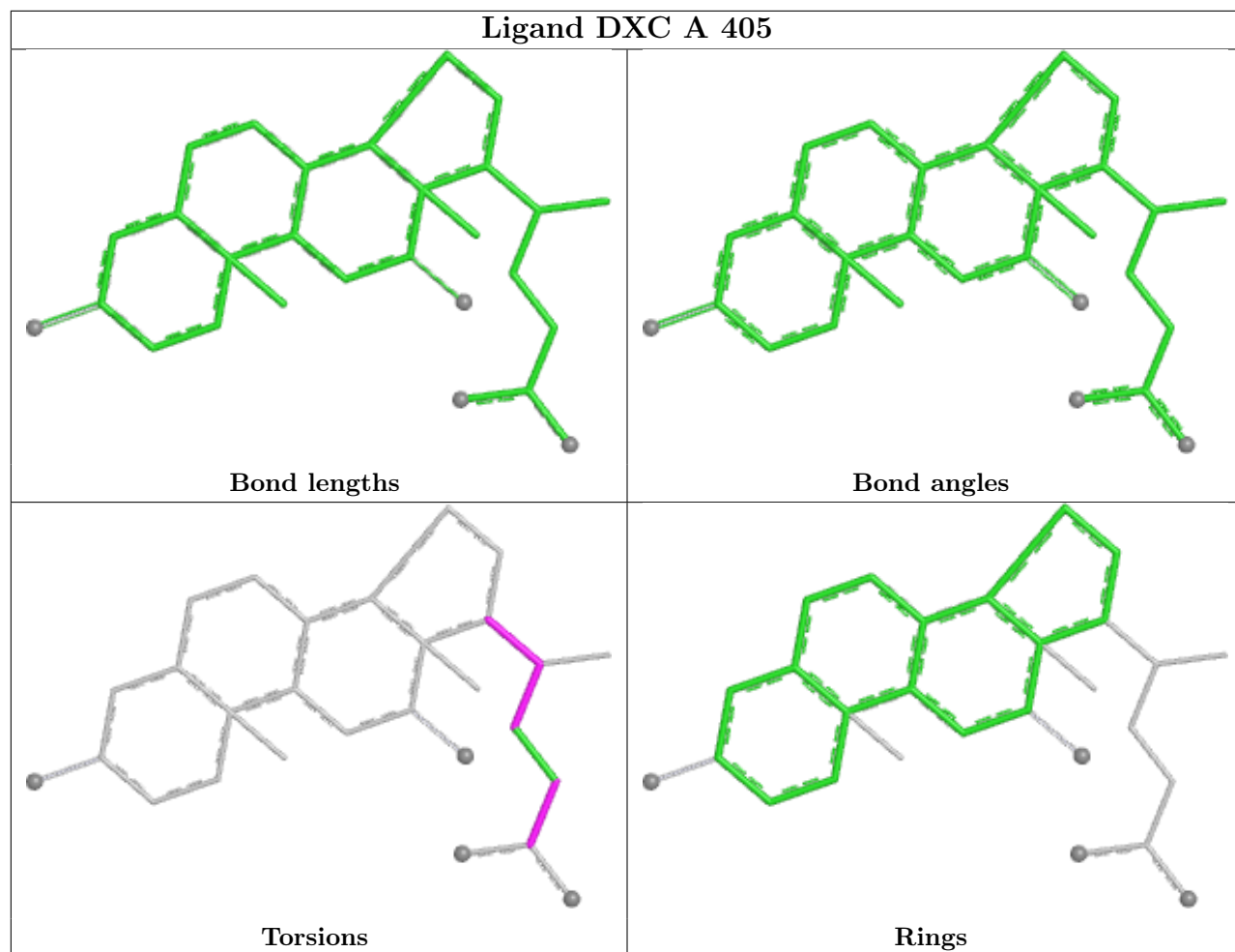
10 monomers are involved in 18 short contacts:

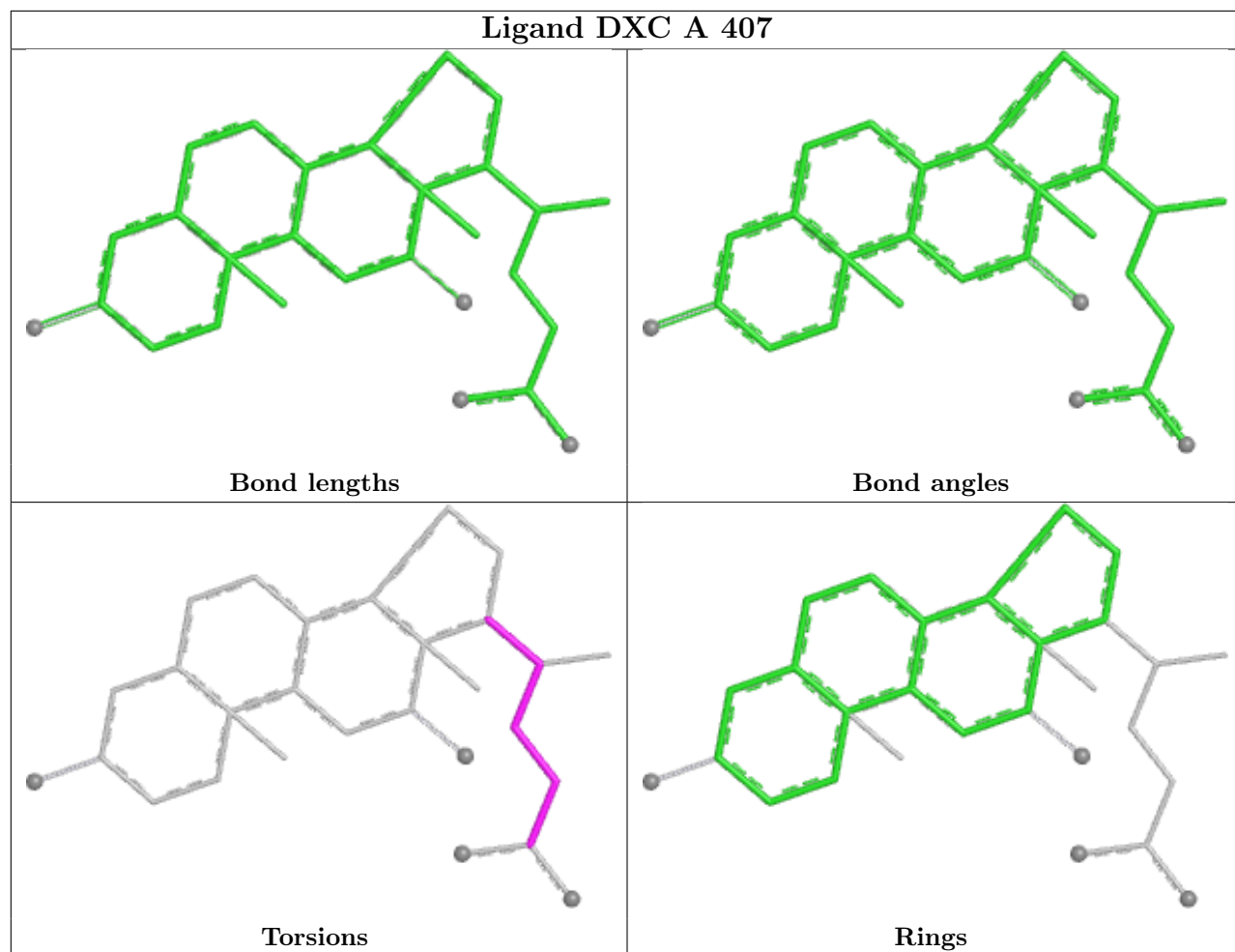
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	609	DXC	1	0
4	A	405	DXC	5	0
4	A	407	DXC	3	0
5	B	610	XBE	3	0
4	B	606	DXC	2	0
4	B	607	DXC	1	0
4	B	601	DXC	1	0
4	A	406	DXC	2	0
4	B	602	DXC	5	0
3	A	403	3PE	2	0

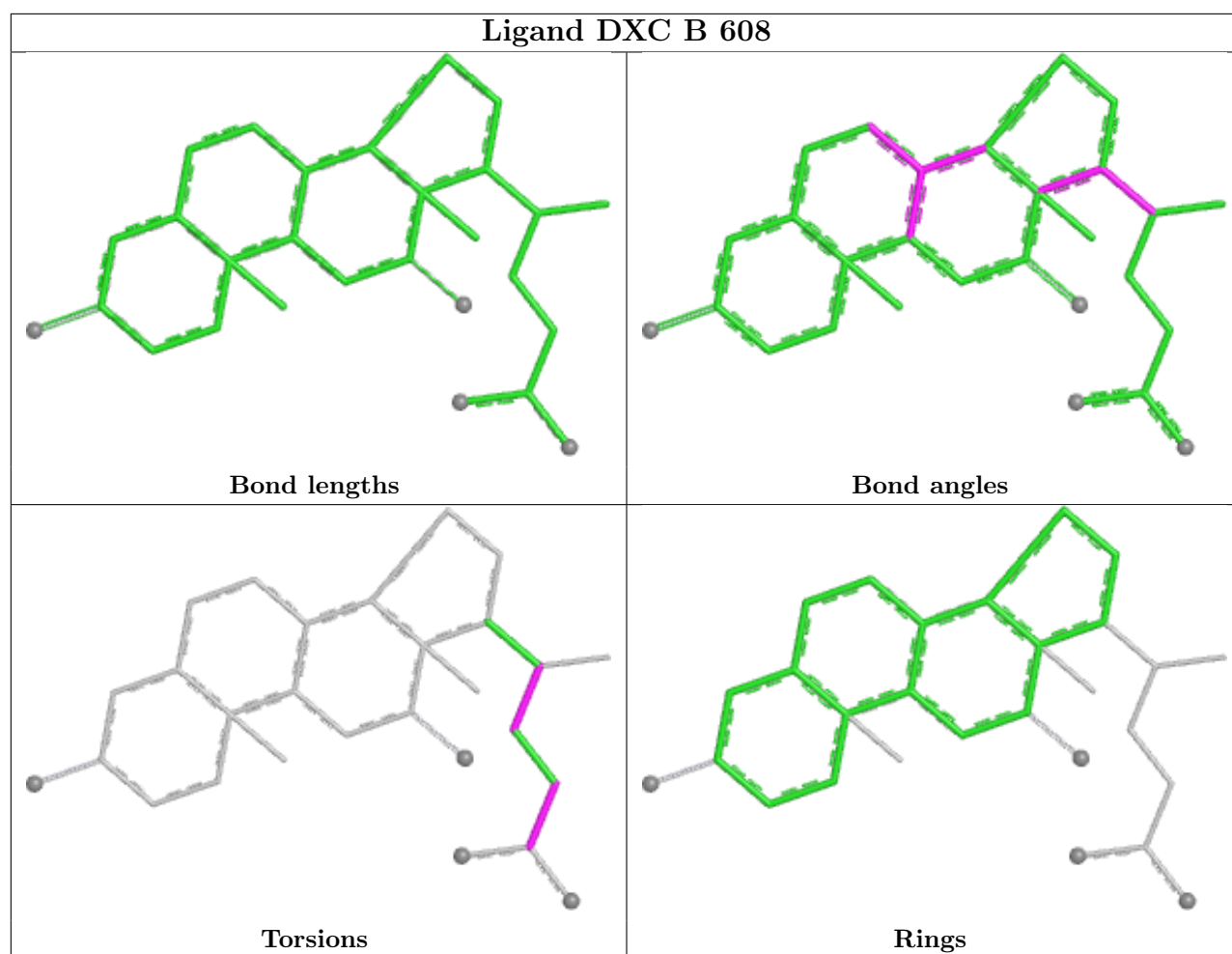
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

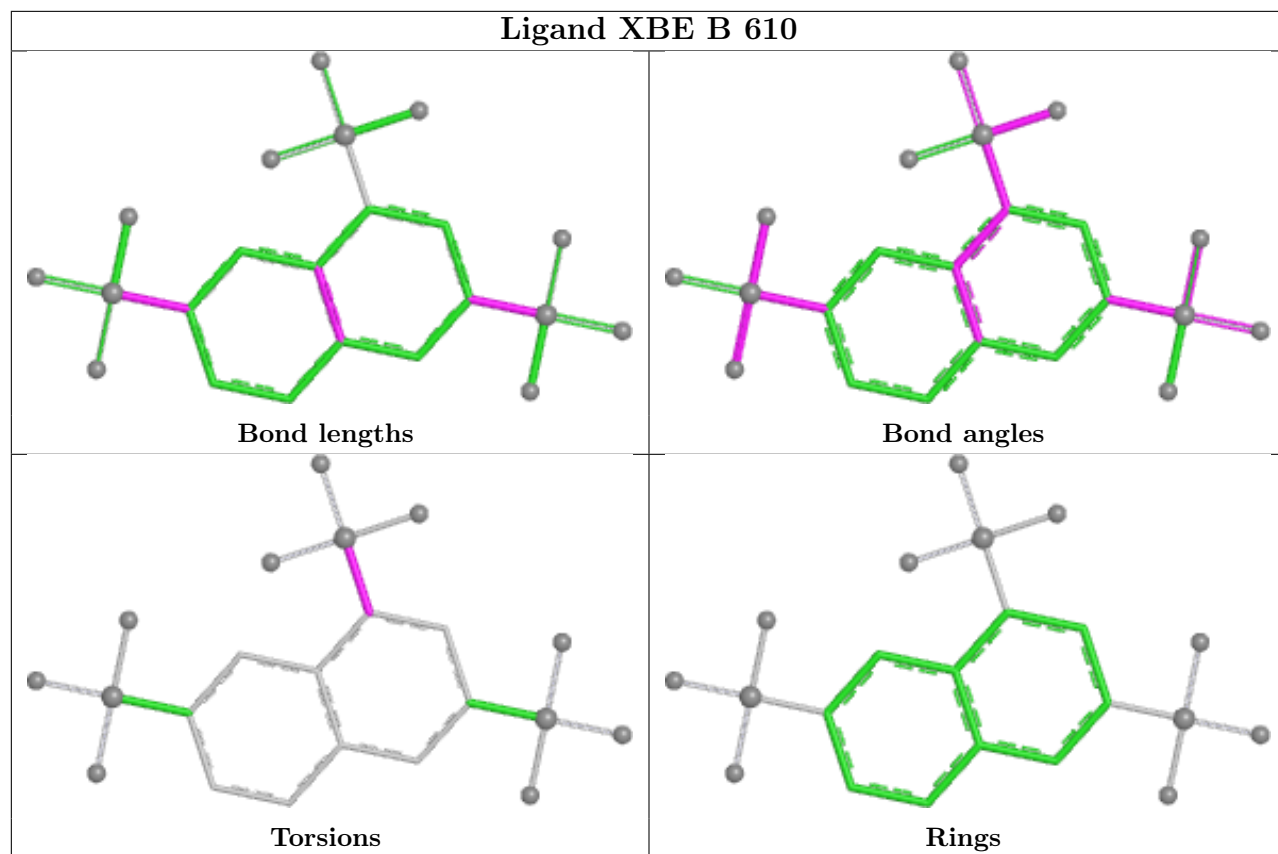
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

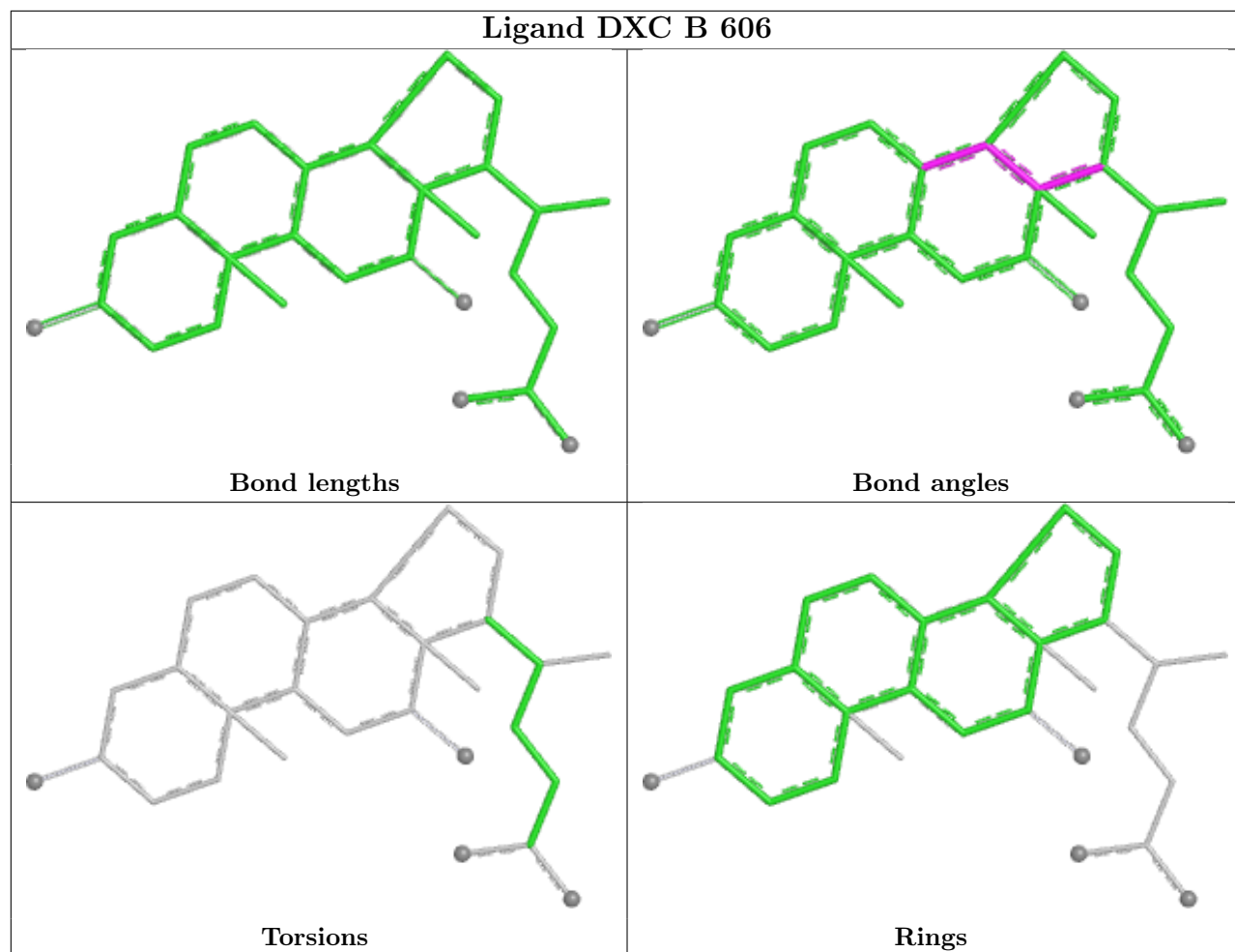


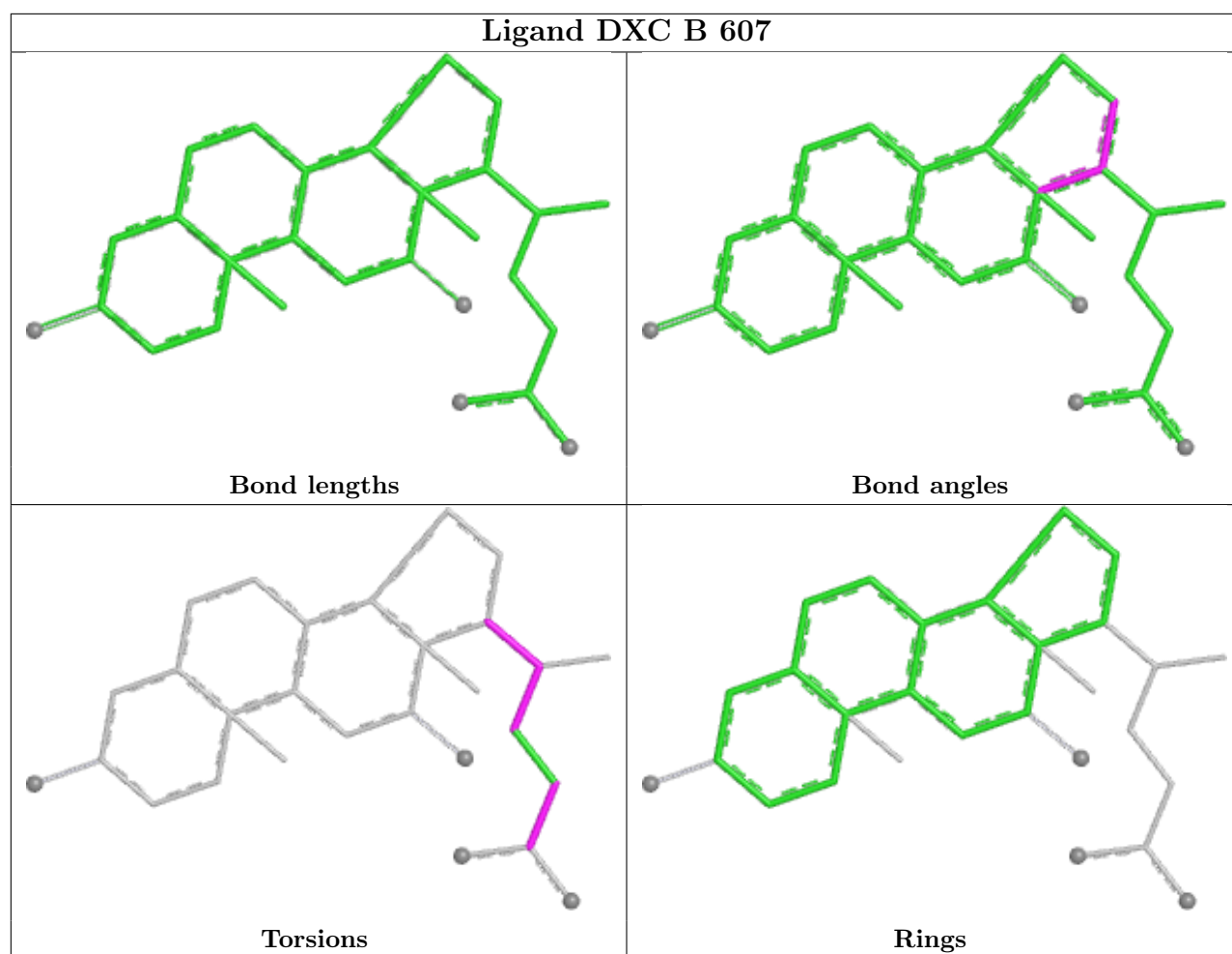


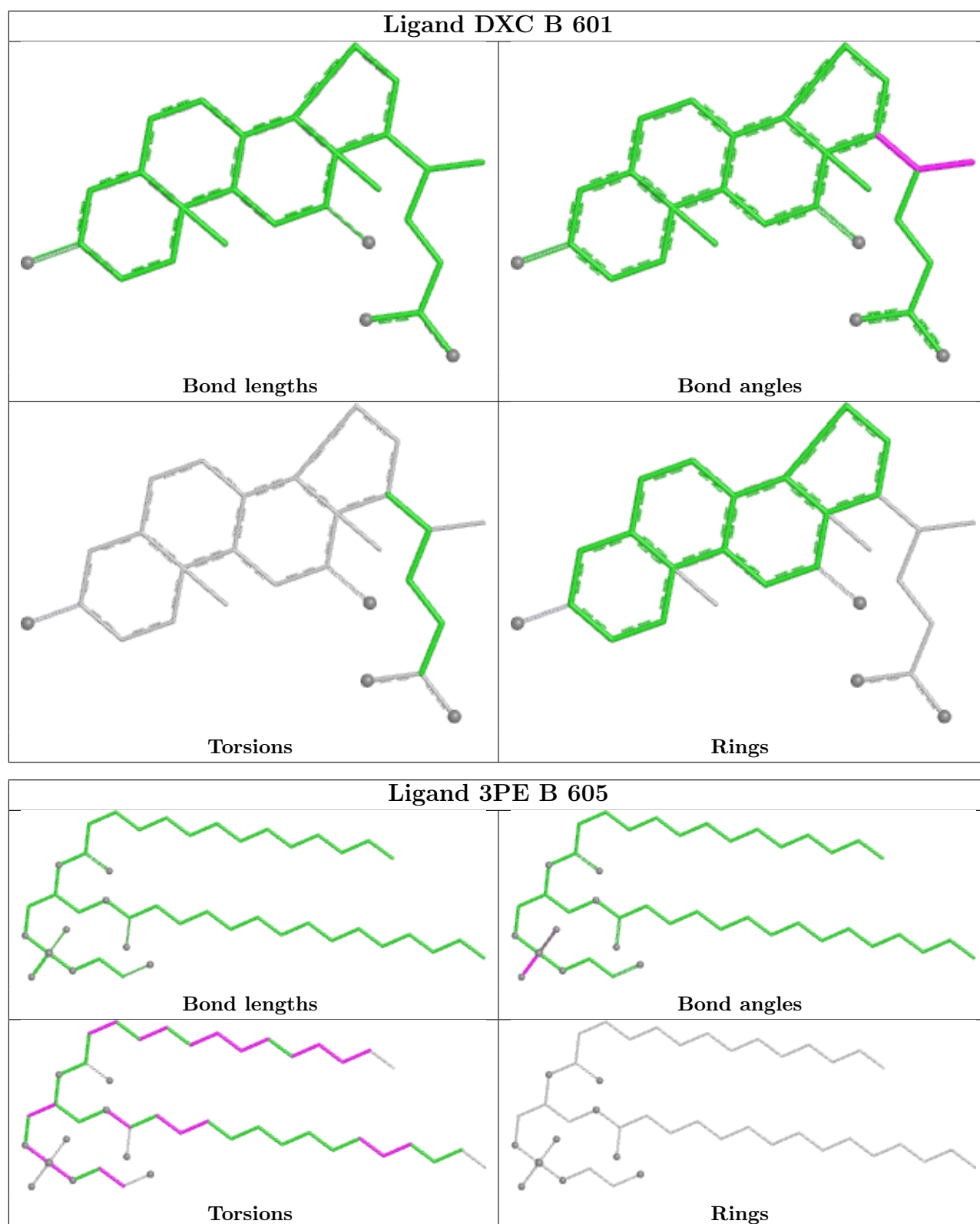


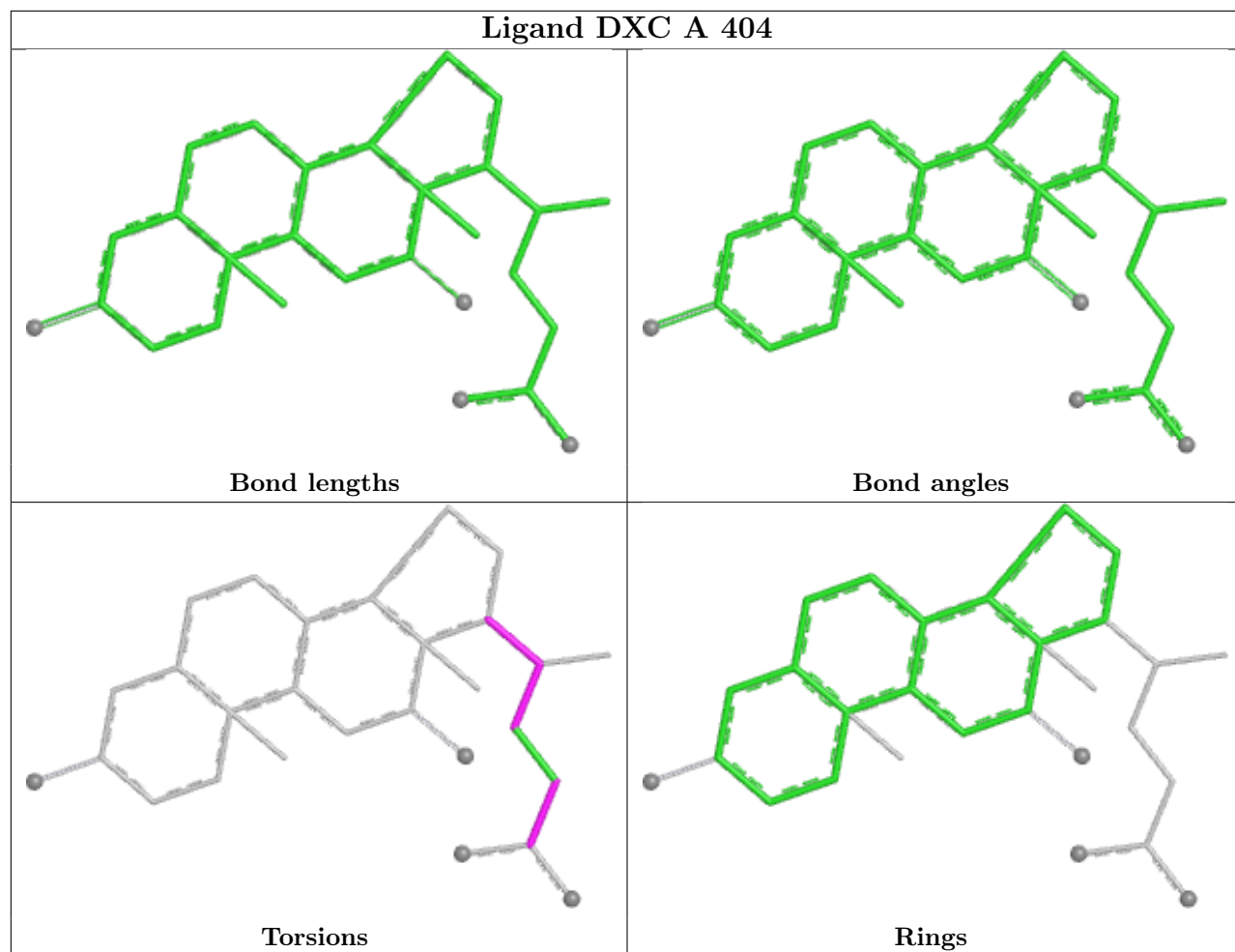


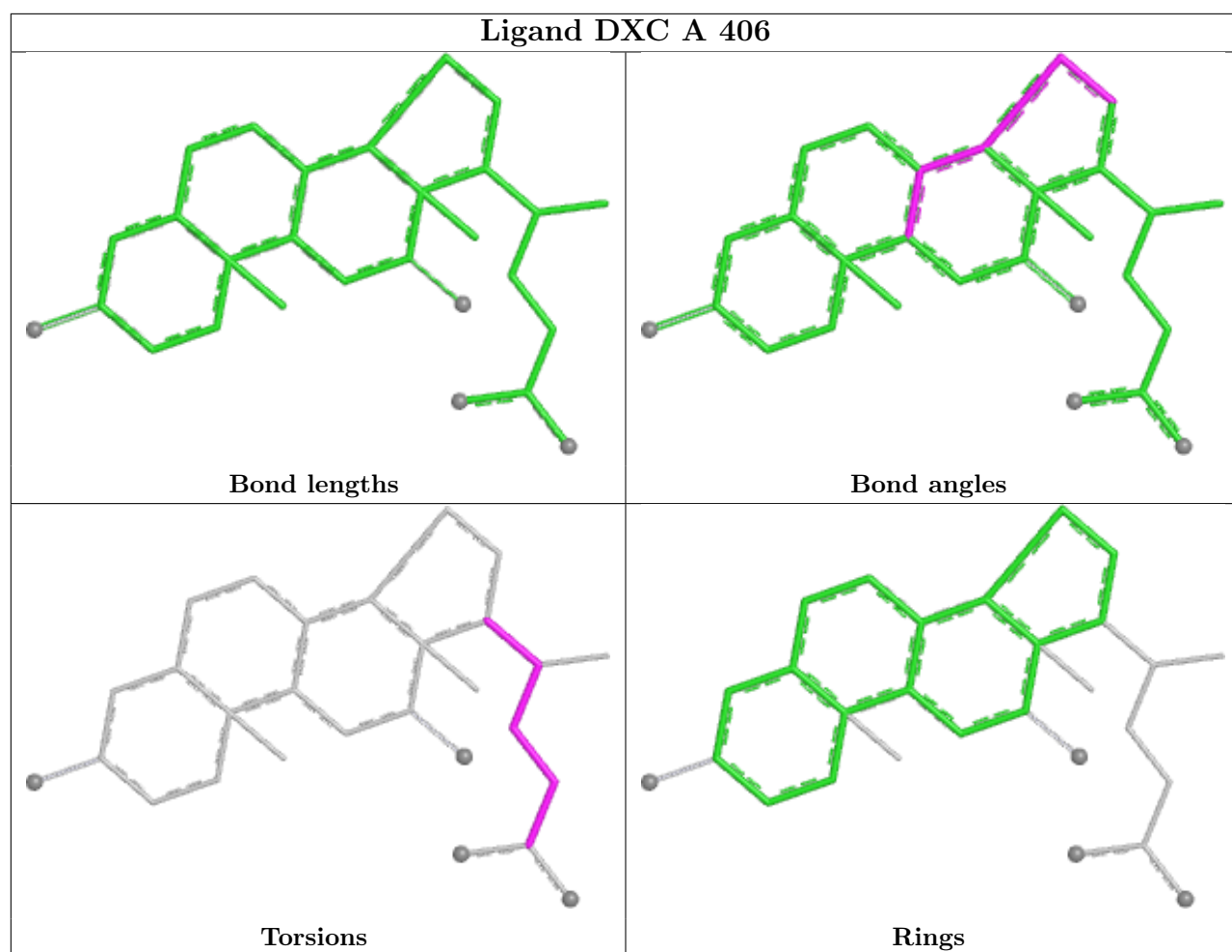


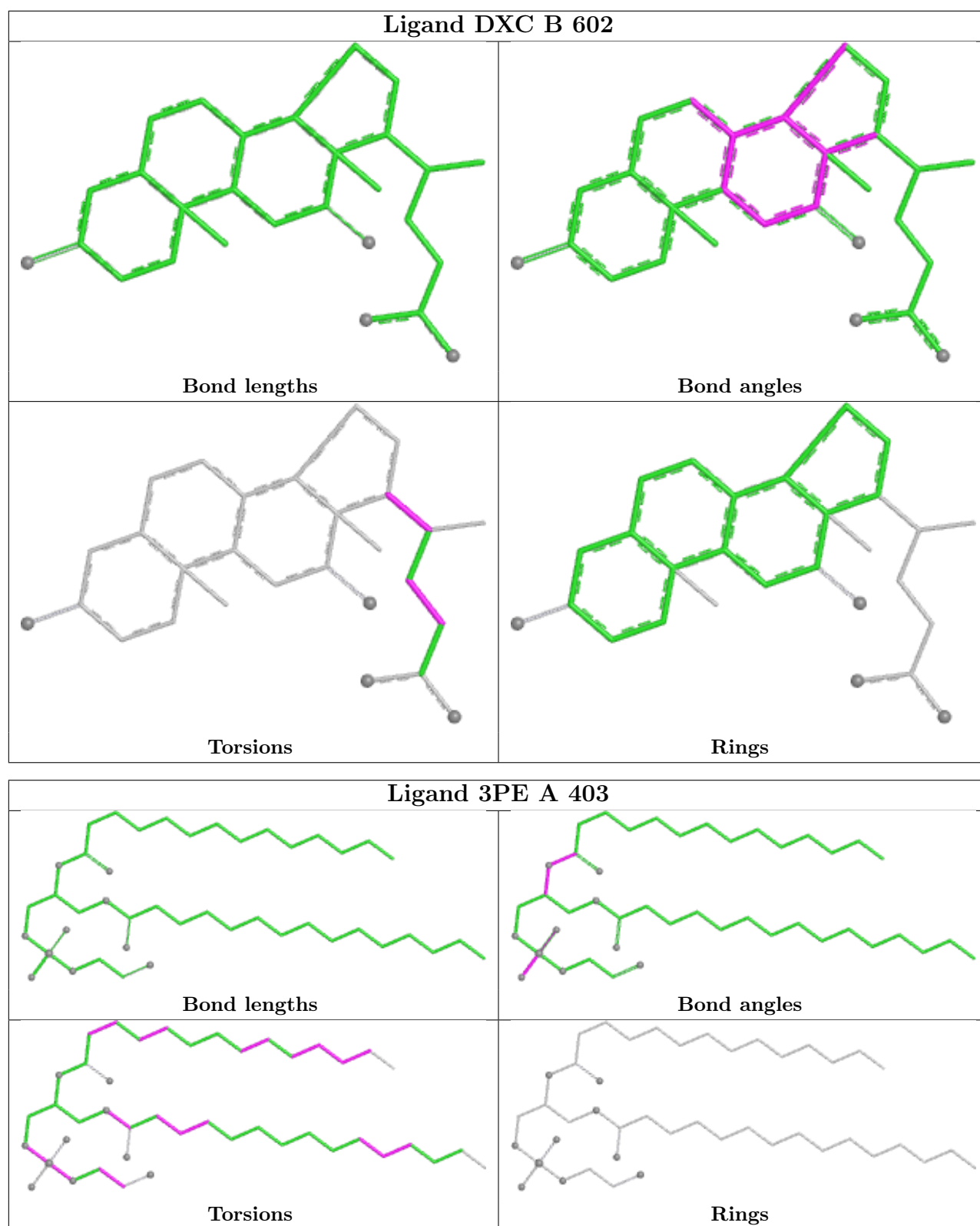












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	332/393 (84%)	0.69	35 (10%) 11 9	47, 91, 153, 197	3 (0%)
1	B	334/393 (84%)	0.50	29 (8%) 16 12	40, 72, 136, 177	3 (0%)
All	All	666/786 (84%)	0.60	64 (9%) 13 11	40, 82, 145, 197	6 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	ASN	10.8
1	B	84	LEU	7.3
1	B	85	ILE	5.9
1	A	80	VAL	5.7
1	B	69	TRP	4.6
1	B	72	TRP	4.5
1	A	81	LEU	4.0
1	B	83	TRP	3.9
1	B	88	LYS	3.8
1	A	84	LEU	3.8
1	A	62	ASP	3.7
1	A	93	VAL	3.7
1	B	66	VAL	3.7
1	A	82	ARG	3.6
1	A	95	SER	3.5
1	A	167[A]	ARG	3.3
1	B	93	VAL	3.3
1	B	167[A]	ARG	3.3
1	A	85	ILE	3.3
1	A	386	LEU	3.3
1	A	94	PRO	3.3
1	A	83	TRP	3.2
1	B	68	PRO	3.1
1	B	59	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	316	PHE	2.9
1	A	90	HIS	2.9
1	B	116[A]	GLU	2.8
1	A	60	GLY	2.8
1	A	73	LYS	2.8
1	A	250	PRO	2.8
1	B	89	ASP	2.8
1	A	72	TRP	2.7
1	B	71	THR	2.7
1	B	178	ILE	2.7
1	B	74	ASN	2.6
1	A	69	TRP	2.5
1	B	73	LYS	2.5
1	A	318	LYS	2.4
1	B	340	MET	2.4
1	A	146	THR	2.4
1	A	66	VAL	2.4
1	A	65	PHE	2.4
1	B	232	TRP	2.4
1	A	88	LYS	2.4
1	A	320	GLN	2.4
1	B	65	PHE	2.3
1	B	103	GLU	2.3
1	A	136	MET	2.3
1	B	316	PHE	2.2
1	A	92	SER	2.2
1	B	81	LEU	2.2
1	A	340	MET	2.2
1	B	80	VAL	2.2
1	B	86	MET	2.2
1	B	87	GLU	2.2
1	A	306	ILE	2.1
1	B	268	GLY	2.1
1	B	325	GLU	2.1
1	A	260	MET	2.1
1	A	321	HIS	2.1
1	B	90	HIS	2.1
1	A	63	GLY	2.0
1	A	118	ALA	2.0
1	A	97	LYS	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](#)

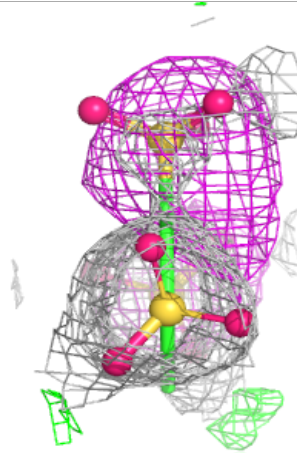
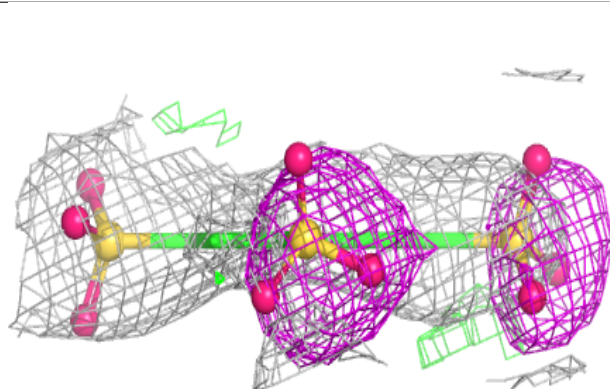
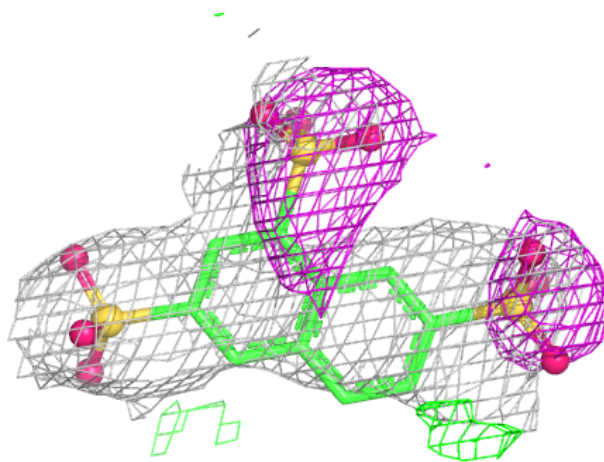
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	XBE	B	610	22/22	0.72	0.18	94,114,119,151	0
4	DXC	B	609	28/28	0.76	0.20	94,106,127,145	0
4	DXC	A	407	28/28	0.82	0.17	106,116,147,161	0
4	DXC	A	406	28/28	0.89	0.19	96,100,110,113	28
4	DXC	B	607	28/28	0.90	0.13	62,67,88,96	0
4	DXC	A	404	28/28	0.91	0.13	61,68,83,97	0
4	DXC	B	608	28/28	0.91	0.15	79,86,110,112	0
4	DXC	A	405	28/28	0.93	0.11	66,77,89,95	0
4	DXC	B	606	28/28	0.93	0.14	56,66,76,80	0
3	3PE	A	403	44/51	0.94	0.14	65,80,87,93	0
4	DXC	B	602	28/28	0.95	0.12	65,71,76,79	28
3	3PE	B	605	44/51	0.95	0.14	58,70,77,80	0
4	DXC	B	601	28/28	0.95	0.12	58,68,77,79	0
2	ZN	A	402	1/1	0.99	0.05	75,75,75,75	0
2	ZN	B	603	1/1	0.99	0.11	62,62,62,62	0
2	ZN	B	604	1/1	0.99	0.07	66,66,66,66	0
2	ZN	A	401	1/1	0.99	0.06	71,71,71,71	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.

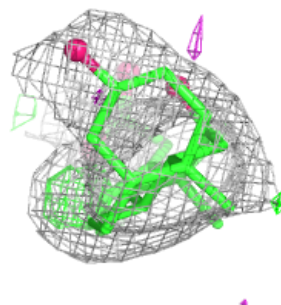
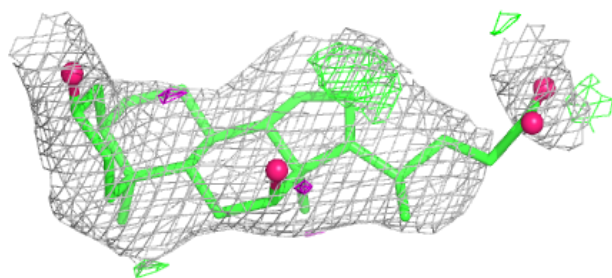
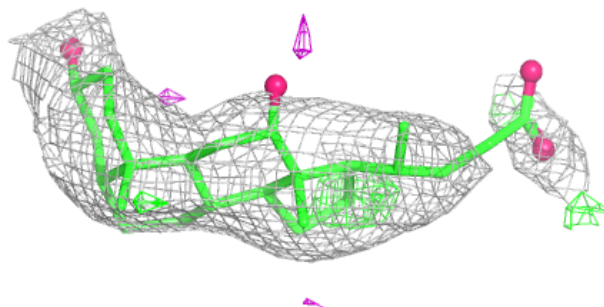
Electron density around XBE B 610:

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

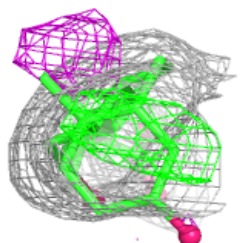
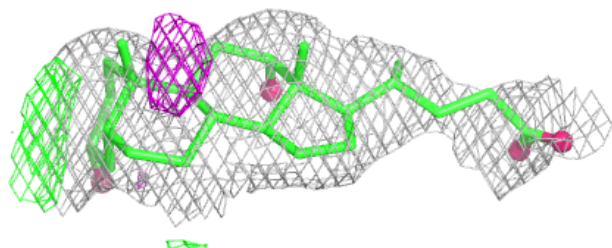
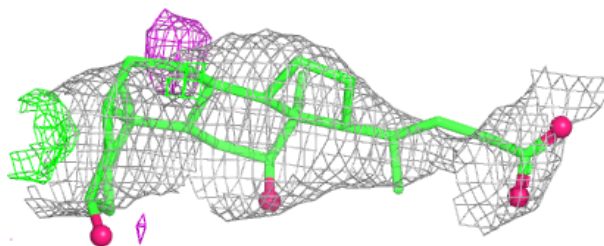


Electron density around DXC B 609:

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

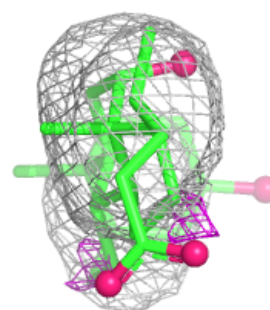
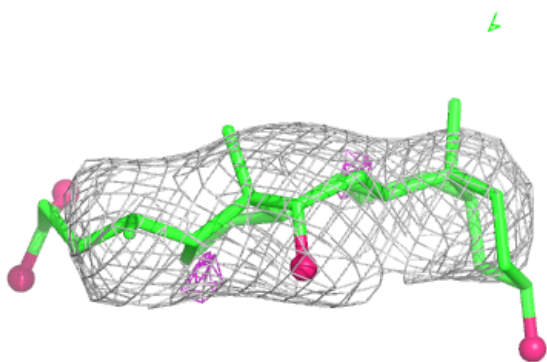
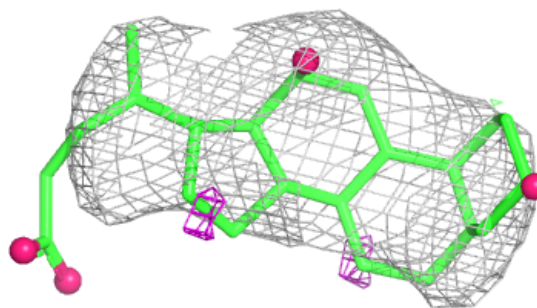
**Electron density around DXC A 407:**

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

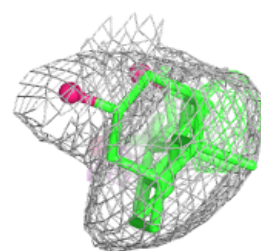
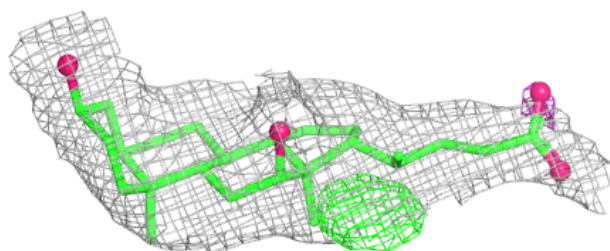
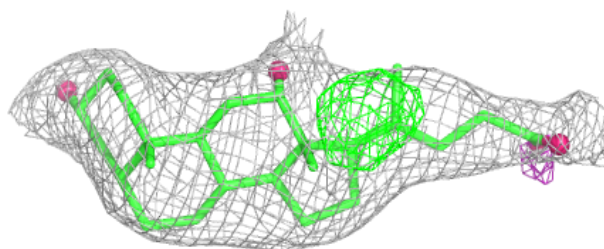


Electron density around DXC A 406:

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

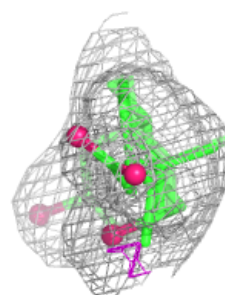
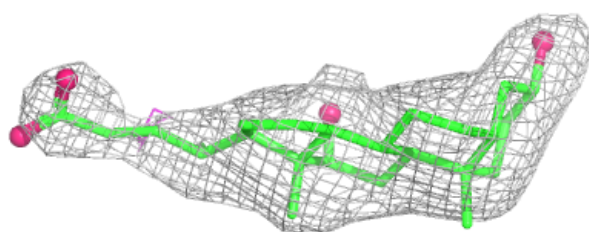
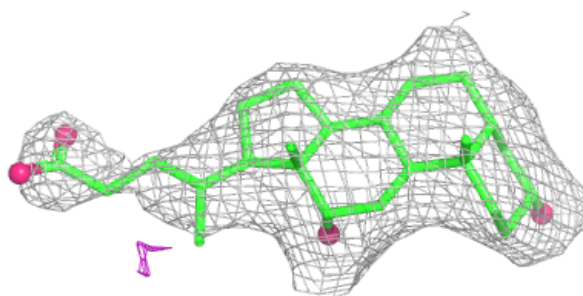
**Electron density around DXC B 607:**

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

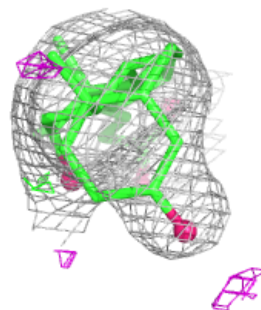
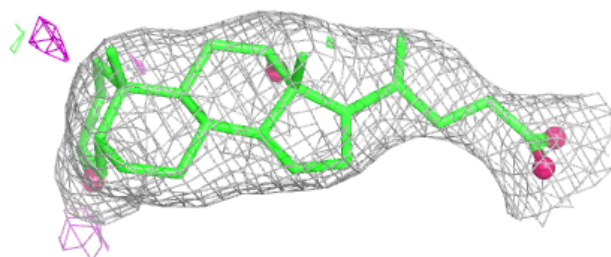
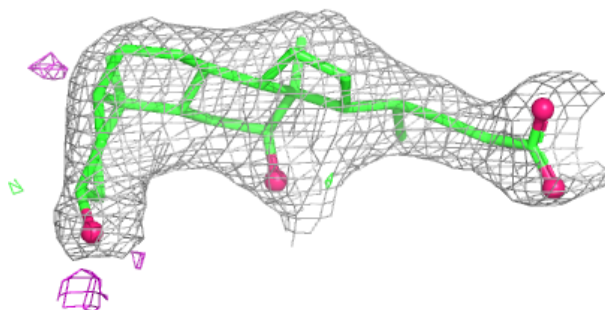


Electron density around DXC A 404:

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

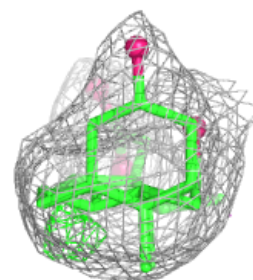
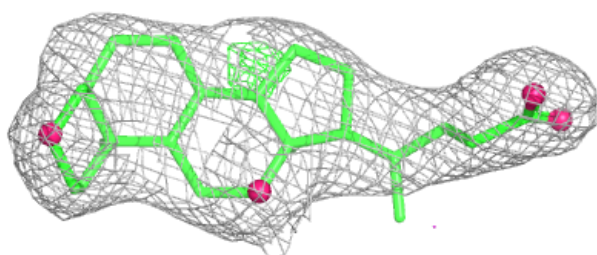
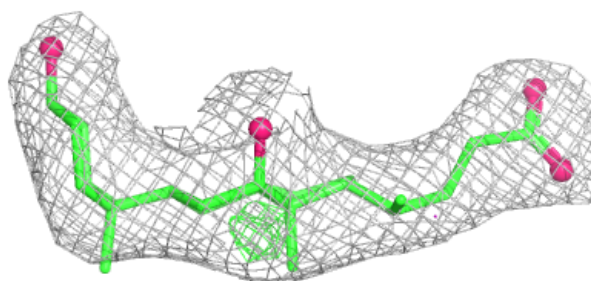
**Electron density around DXC B 608:**

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

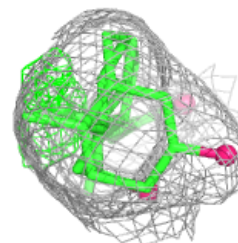
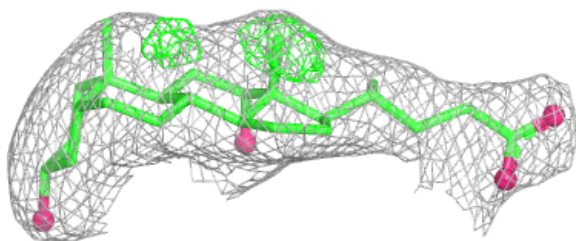
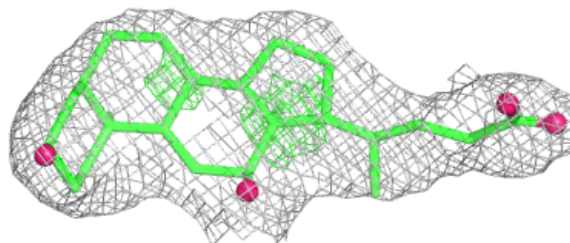


Electron density around DXC A 405:

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

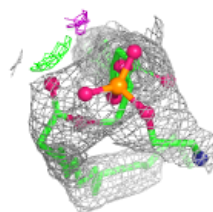
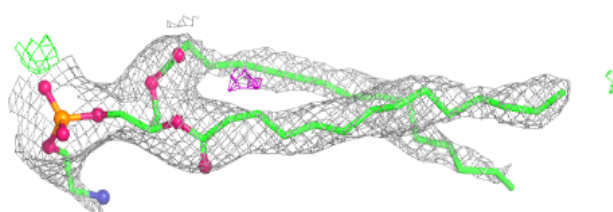
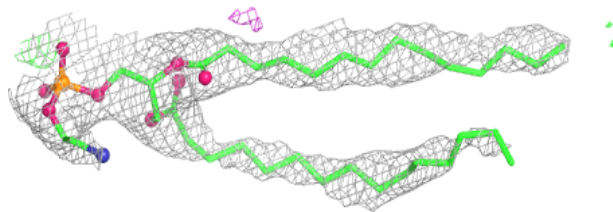
**Electron density around DXC B 606:**

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

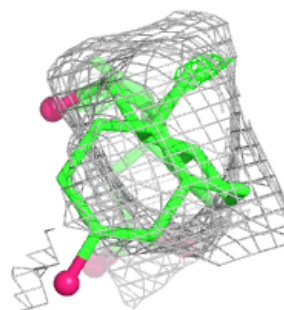
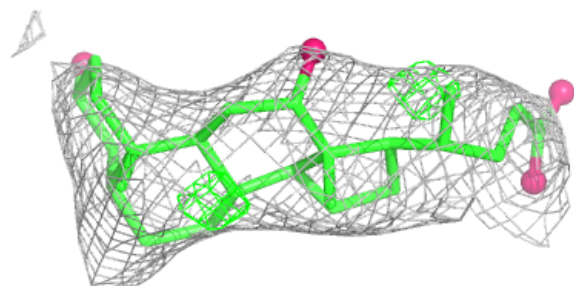
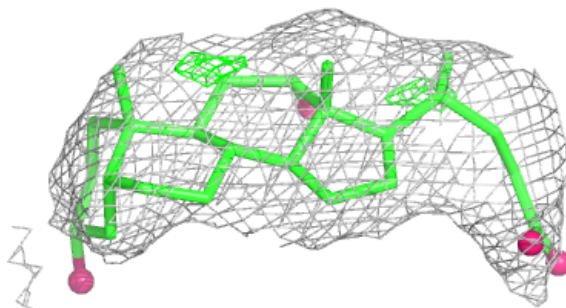


Electron density around 3PE A 403:

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

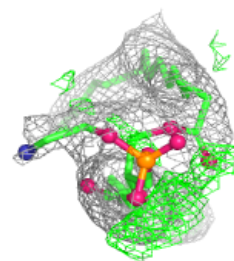
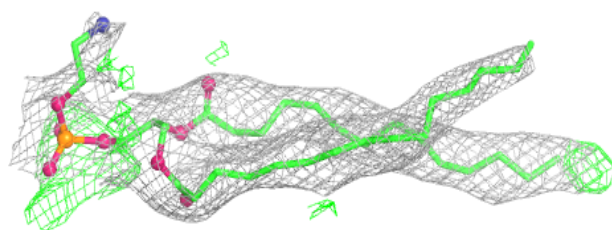
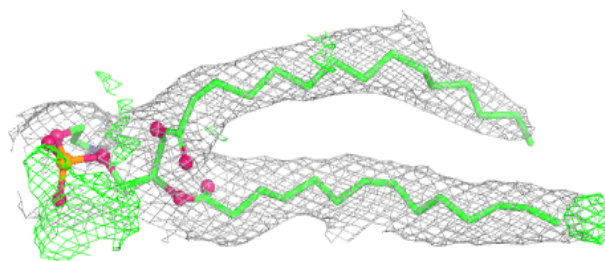
**Electron density around DXC B 602:**

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

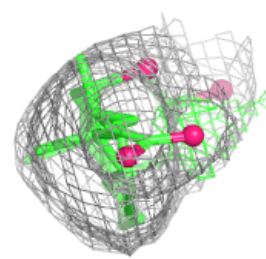
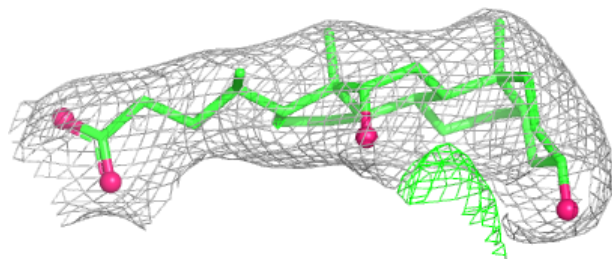
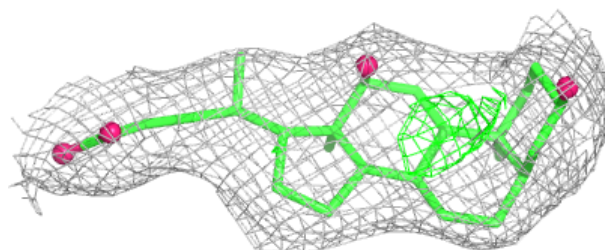


Electron density around 3PE B 605:

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

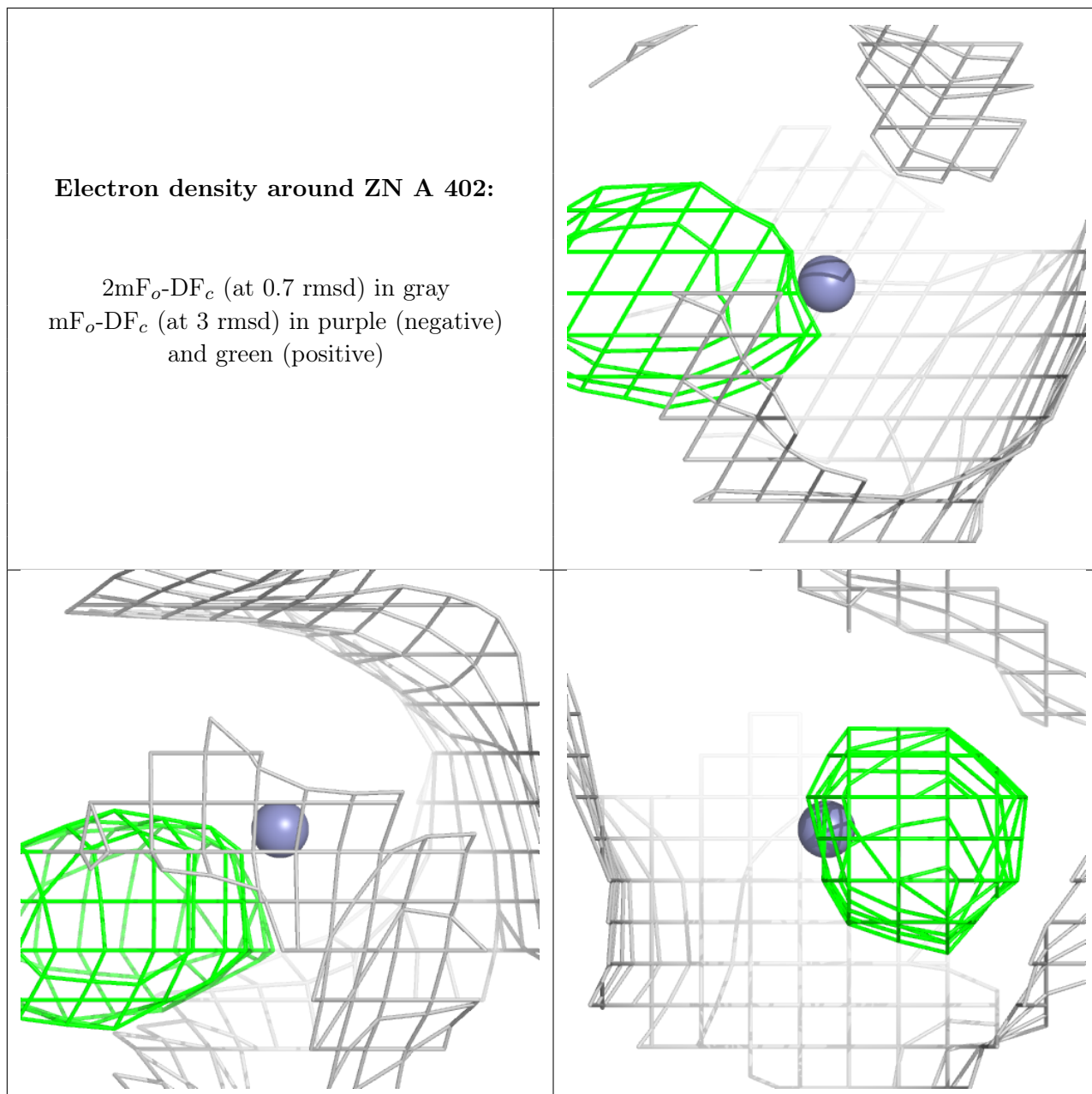
**Electron density around DXC B 601:**

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



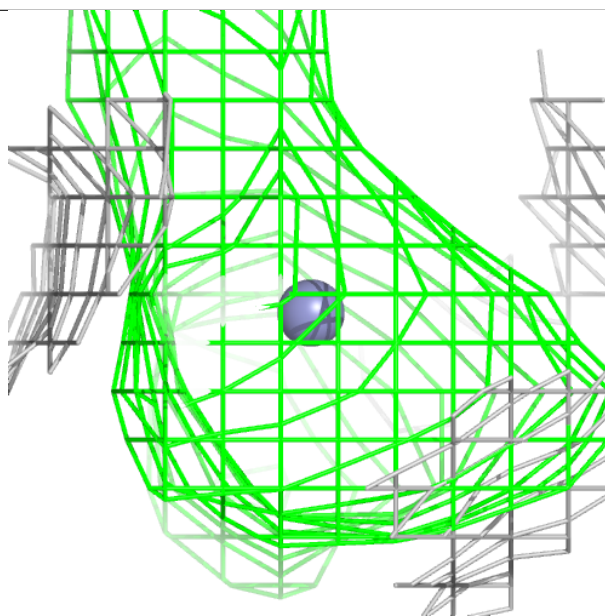
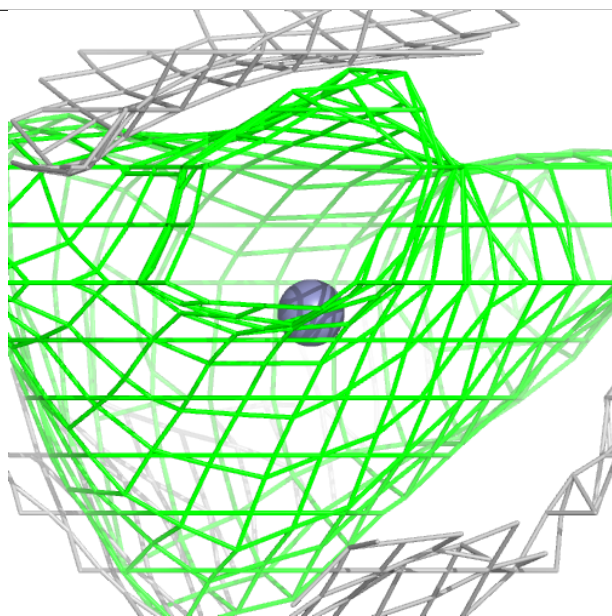
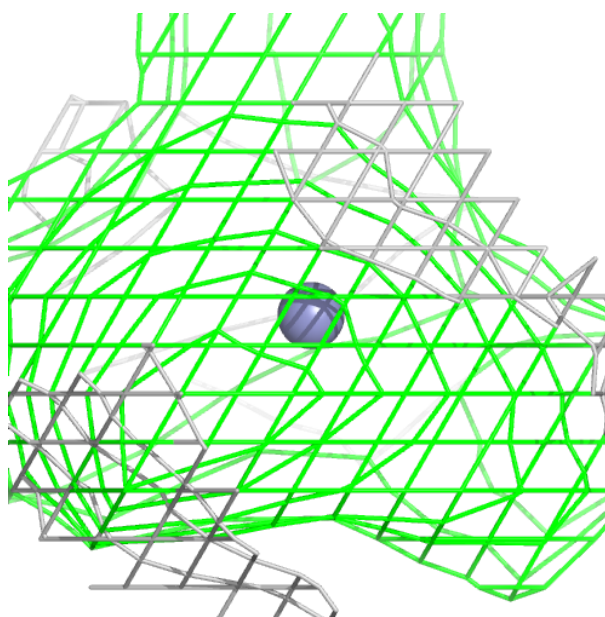
Electron density around ZN A 402:

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



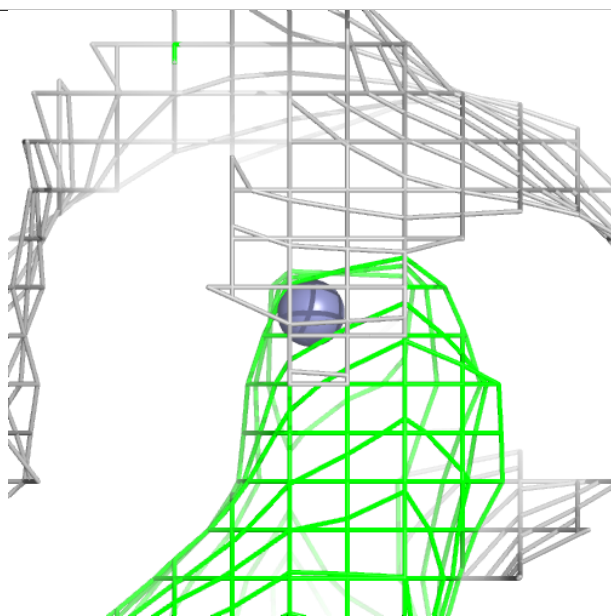
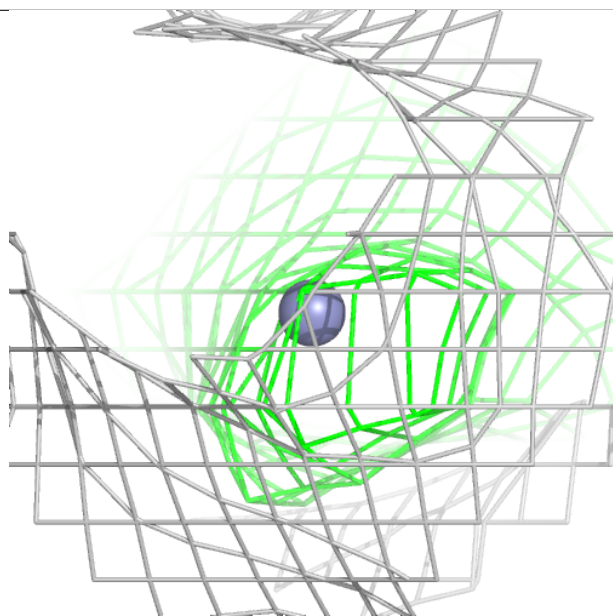
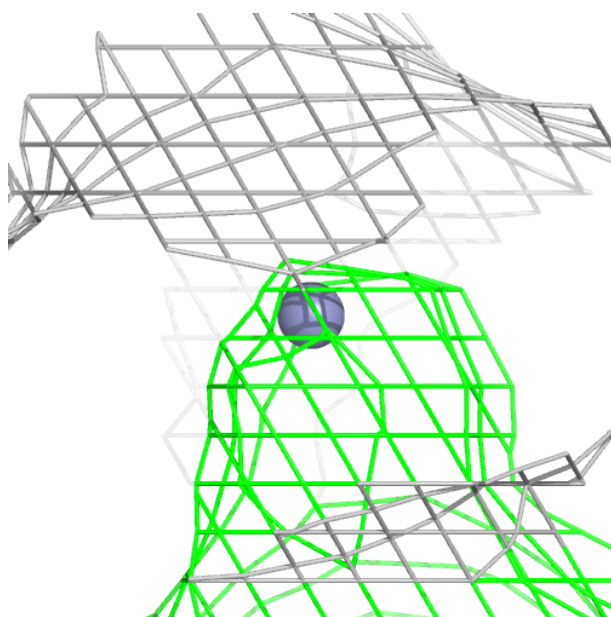
Electron density around ZN B 603:

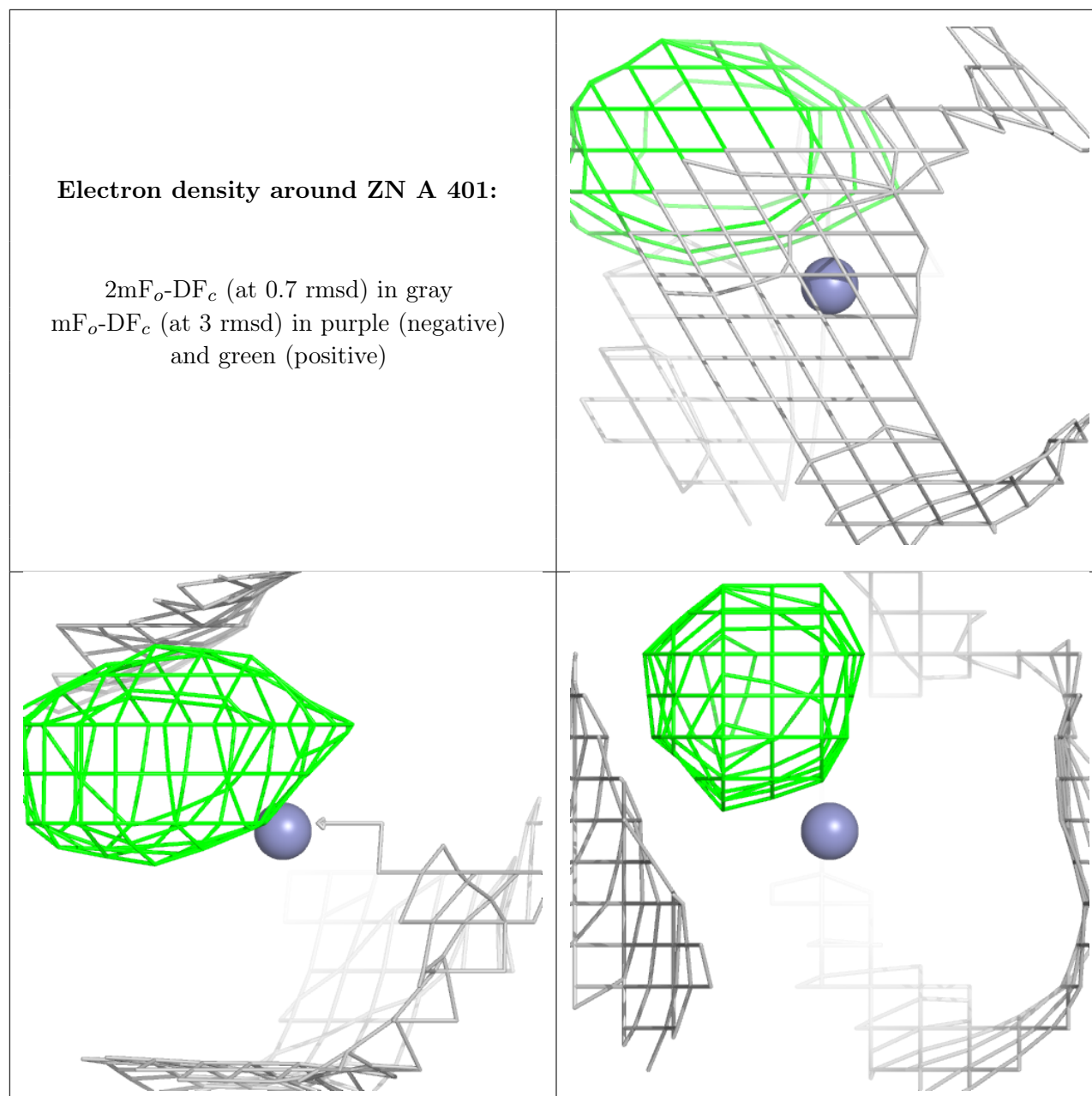
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN B 604:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.