



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:49 PM UTC

PDB ID : 8PC4 / pdb_00008pc4
Title : MEMBRANE TARGET COMPLEX 1
Authors : Garau, G.
Deposited on : 2023-06-09
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 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

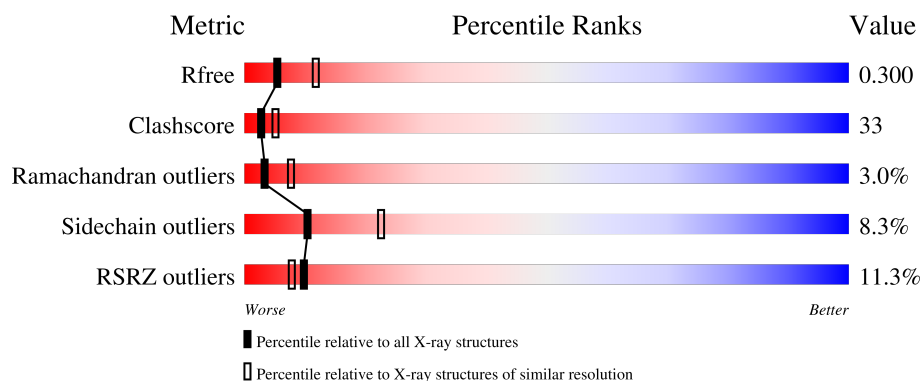
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	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	10% 37% 39% 7% 16%
1	B	393	9% 43% 37% 15%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5928 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.

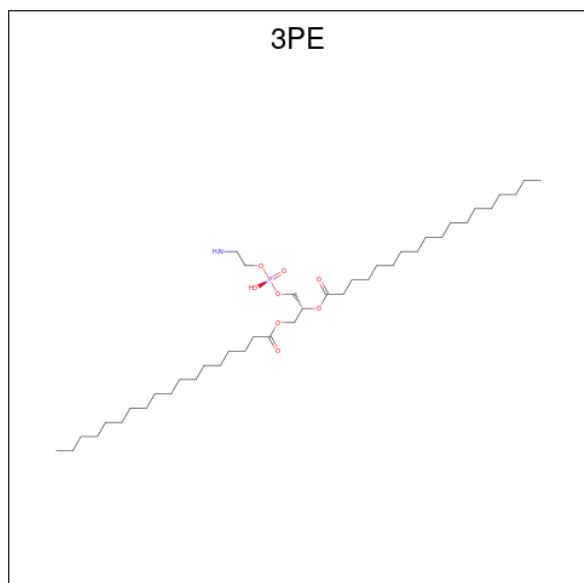
- Molecule 1 is a protein called N-acyl-phosphatidylethanolamine-hydrolyzing phospholipase D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	3	0
			2752	1785	467	486	14			
1	B	334	Total	C	N	O	S	0	3	0
			2749	1776	465	494	14			

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

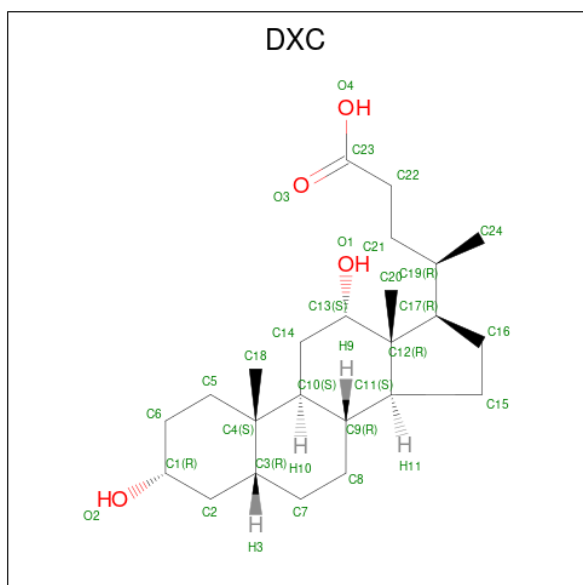
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- 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).



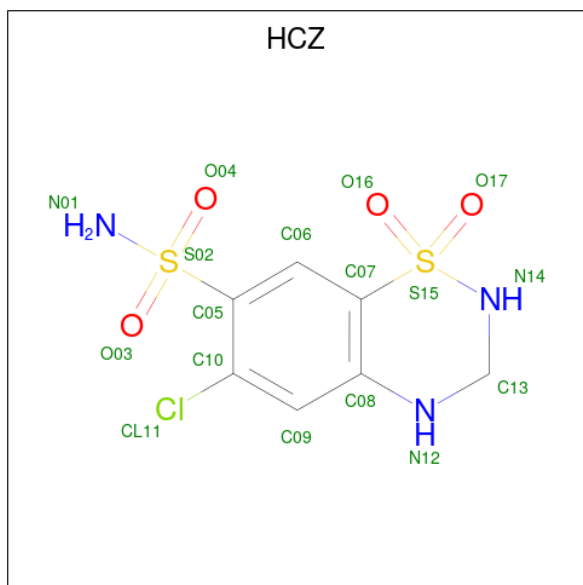
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24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

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

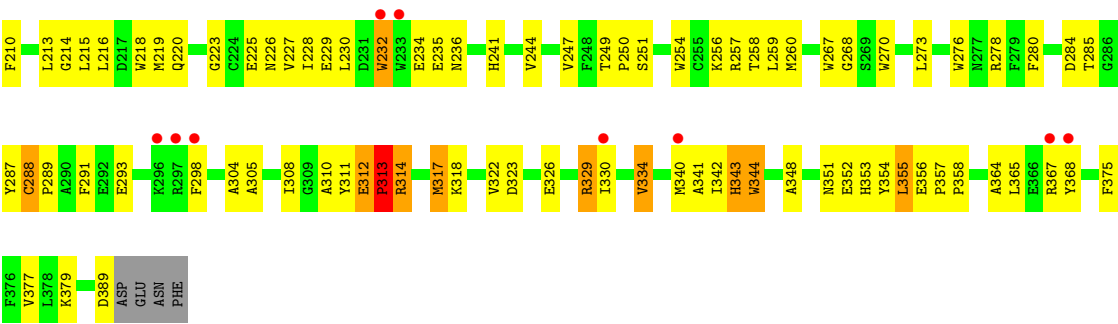
- Molecule 5 is 6-chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide (CCD ID: HCZ) (formula: C₇H₈ClN₃O₄S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	S	0	0
			17	7	1	3	4	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total	O	0	0
			16	16		
6	B	22	Total	O	0	0
			22	22		



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	94.39Å 94.39Å 442.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.75 – 2.85 54.75 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (54.75-2.85) 99.5 (54.75-2.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.265 , 0.301 0.264 , 0.300	Depositor DCC
R_{free} test set	1797 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	87.8	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 90.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5928	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: ZN, 3PE, HCZ, DXC

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	0.53	2/2858 (0.1%)	0.77	4/3892 (0.1%)
1	B	0.42	0/2851	0.74	1/3881 (0.0%)
All	All	0.48	2/5709 (0.0%)	0.75	5/7773 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315[A]	TRP	C-O	6.89	1.32	1.24
1	A	315[B]	TRP	C-O	6.89	1.32	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ARG	N-CA-C	-5.64	106.79	113.38
1	A	315[A]	TRP	CA-C-O	5.52	128.40	120.51
1	A	315[B]	TRP	CA-C-O	5.52	128.40	120.51
1	B	313	PRO	CA-N-CD	-5.27	104.63	112.00
1	A	68	PRO	CA-N-CD	-5.25	104.64	112.00

There are no chirality outliers.

There are no planarity outliers.

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	2752	0	2651	213	0
1	B	2749	0	2641	160	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	62	8	0
3	B	44	0	62	5	0
4	A	168	0	234	21	0
4	B	112	0	156	9	0
5	B	17	0	8	1	0
6	A	16	0	0	0	0
6	B	22	0	0	0	0
All	All	5928	0	5814	389	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 33.

All (389) 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:312:GLU:HG3	1:B:313:PRO:CD	1.80	1.11
1:B:312:GLU:HG3	1:B:313:PRO:HD2	1.31	1.09
1:B:73:LYS:HG2	1:B:288:CYS:HB2	1.45	0.95
1:A:326:GLU:HA	1:A:329:ARG:HG3	1.49	0.94
1:B:323:ASP:OD1	1:B:326:GLU:HG3	1.73	0.89
1:B:312:GLU:CG	1:B:313:PRO:HD2	2.01	0.89
1:A:142:LEU:CD2	1:A:144:PHE:HD2	1.89	0.86
1:A:82:ARG:HG2	4:A:409:DXC:H51	1.59	0.85
1:A:236:ASN:OD1	1:A:237:CYS:N	2.10	0.84
1:A:371:ASN:OD1	1:A:373:GLU:HG3	1.81	0.81
1:A:59:LYS:HE3	1:A:293:GLU:HB3	1.63	0.80
4:A:405:DXC:H211	4:B:602:DXC:H81	1.63	0.79
1:B:136:MET:HE1	1:B:176:PRO:HG2	1.64	0.79
1:B:365:LEU:HD11	1:B:375:PHE:HB3	1.62	0.78
1:A:69:TRP:HD1	1:A:266:LEU:HD13	1.48	0.78
1:A:142:LEU:HD22	1:A:144:PHE:HD2	1.48	0.77
1:A:258:THR:HA	3:A:403:3PE:H282	1.67	0.77
1:A:67:ASN:OD1	1:A:68:PRO:HD3	1.85	0.76
1:B:312:GLU:HG2	1:B:351:ASN:HB3	1.67	0.76
1:A:101:ASP:HA	1:A:166:ARG:HH22	1.51	0.76
1:B:65:PHE:HB2	1:B:70:PRO:HG3	1.65	0.76
1:A:314:ARG:HB3	1:A:318:LYS:HE3	1.68	0.75
1:A:83:TRP:HE1	1:A:88:LYS:HA	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLU:O	1:A:241:HIS:CD2	2.39	0.74
1:A:314:ARG:O	1:A:318:LYS:HG2	1.89	0.72
1:A:371:ASN:ND2	1:A:374:ASP:OD1	2.23	0.72
1:A:254:TRP:HA	1:A:267:TRP:CZ3	2.25	0.72
1:B:60:GLY:HA3	1:B:72:TRP:CZ3	2.25	0.71
1:A:126:ARG:HD2	1:A:138:GLU:OE2	1.90	0.71
1:A:97:LYS:HD3	1:A:101:ASP:OD1	1.91	0.70
1:A:75:PRO:HB2	1:A:252:GLN:HE22	1.56	0.70
1:A:62:ASP:HA	1:A:232:TRP:HE1	1.55	0.70
1:B:322:VAL:HB	1:B:326:GLU:HB2	1.71	0.70
1:B:136:MET:HE2	1:B:143:ILE:HG21	1.74	0.69
1:B:312:GLU:HG3	1:B:313:PRO:HD3	1.73	0.69
1:A:326:GLU:HA	1:A:329:ARG:CG	2.21	0.69
1:A:314:ARG:HE	1:A:314:ARG:HA	1.56	0.69
1:B:67:ASN:H	1:B:68:PRO:HD2	1.57	0.69
1:B:287:TYR:HD1	1:B:288:CYS:N	1.90	0.69
1:A:120:VAL:HG21	1:A:139:MET:HA	1.75	0.68
1:B:127:VAL:HG21	1:B:340:MET:HE1	1.76	0.67
1:A:141:GLU:O	1:A:241:HIS:HD2	1.76	0.67
1:A:241:HIS:ND1	1:A:241:HIS:N	2.43	0.67
1:B:172:ILE:O	1:B:175:LEU:HG	1.94	0.66
1:A:69:TRP:CD1	1:A:266:LEU:HD13	2.28	0.66
1:B:312:GLU:O	1:B:313:PRO:C	2.38	0.66
1:A:89:ASP:OD1	1:A:90:HIS:N	2.29	0.65
1:B:312:GLU:CB	1:B:313:PRO:HD2	2.27	0.64
1:A:317:MET:HE1	3:A:403:3PE:H122	1.80	0.64
1:B:232:TRP:CH2	1:B:250:PRO:HA	2.32	0.64
1:B:73:LYS:HG3	1:B:289:PRO:HD2	1.79	0.64
1:B:125:LEU:CD2	1:B:139:MET:HB3	2.27	0.63
1:B:251:SER:HB3	1:B:268:GLY:HA2	1.80	0.63
4:A:405:DXC:H211	4:B:602:DXC:H151	1.80	0.63
1:B:59:LYS:HA	1:B:293:GLU:OE1	1.97	0.63
1:B:149:ILE:HD12	1:B:192:ASP:HB2	1.79	0.63
1:A:254:TRP:HA	1:A:267:TRP:CE3	2.34	0.63
1:B:364:ALA:HA	1:B:367:ARG:HD3	1.81	0.63
1:B:235:GLU:HB3	1:B:247:VAL:HG22	1.81	0.63
1:A:347:PHE:HB2	1:A:349:LEU:HD11	1.80	0.62
1:A:243:LYS:H	1:A:243:LYS:HD2	1.62	0.62
1:B:65:PHE:O	1:B:66:VAL:C	2.42	0.62
1:B:80:VAL:O	1:B:82:ARG:NH2	2.32	0.62
1:A:64:ARG:HA	1:A:70:PRO:HD3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LYS:HB3	1:B:75:PRO:HD2	1.82	0.62
1:A:134:THR:HA	1:A:146:THR:O	1.99	0.62
1:A:238:VAL:HG13	1:A:239:PRO:HD2	1.82	0.62
1:B:312:GLU:CG	1:B:313:PRO:CD	2.66	0.61
1:A:111:PHE:CD2	1:A:176:PRO:HD3	2.34	0.61
1:A:81:LEU:HG	4:A:409:DXC:H62	1.83	0.60
1:A:232:TRP:CE3	1:A:250:PRO:HA	2.35	0.60
1:B:134:THR:HG23	1:B:148:PRO:HA	1.83	0.60
1:B:123:ALA:N	1:B:276:TRP:HE1	2.00	0.60
1:B:260:MET:HA	1:B:260:MET:HE3	1.84	0.60
1:A:59:LYS:HG3	1:A:233:TRP:CZ2	2.36	0.59
1:B:355:LEU:O	1:B:358:PRO:HD2	2.02	0.59
1:A:77:ILE:HD12	1:A:319:TYR:CE1	2.38	0.59
1:A:181:VAL:HG21	1:A:209:TRP:CE3	2.37	0.59
1:A:90:HIS:C	1:A:92:SER:H	2.10	0.59
1:B:227:VAL:O	1:B:228:ILE:HD13	2.02	0.58
1:B:200:ASN:ND2	1:B:223:GLY:O	2.37	0.58
1:B:273:LEU:HD12	1:B:278:ARG:HG2	1.86	0.57
1:A:175:LEU:HD13	1:A:178:ILE:HD11	1.85	0.57
4:A:406:DXC:H183	4:A:407:DXC:H203	1.84	0.57
1:A:97:LYS:O	1:A:101:ASP:OD1	2.22	0.57
1:A:126:ARG:HB3	1:A:138:GLU:HG3	1.86	0.57
1:A:360:LYS:HA	1:A:363:GLU:CD	2.30	0.57
1:B:305:ALA:HB1	1:B:342:ILE:HG21	1.86	0.57
1:A:341:ALA:HB2	1:A:375:PHE:HE1	1.68	0.57
4:B:601:DXC:H203	4:B:602:DXC:H182	1.86	0.57
1:A:90:HIS:CD2	1:A:93:VAL:HA	2.40	0.57
1:B:134:THR:HA	1:B:146:THR:O	2.04	0.57
1:B:65:PHE:H	1:B:70:PRO:HD3	1.68	0.56
1:A:192:ASP:O	1:A:196:VAL:HG23	2.05	0.56
1:A:185:HIS:CE1	1:A:190:HIS:CD2	2.93	0.56
1:B:312:GLU:HG2	1:B:351:ASN:CB	2.35	0.56
1:A:303:LEU:HD13	1:A:304:ALA:N	2.21	0.56
1:B:216:LEU:HB2	1:B:229:GLU:CD	2.31	0.56
1:A:216:LEU:HB2	1:A:229:GLU:CD	2.31	0.56
1:B:247:VAL:HG11	1:B:298:PHE:CZ	2.41	0.56
1:A:62:ASP:HA	1:A:232:TRP:NE1	2.20	0.55
1:A:80:VAL:O	1:A:81:LEU:C	2.49	0.55
1:A:82:ARG:CG	4:A:409:DXC:H51	2.32	0.55
1:A:310:ALA:N	1:A:352:GLU:OE2	2.37	0.55
1:B:123:ALA:H	1:B:276:TRP:HE1	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ILE:HG21	1:B:236:ASN:HD22	1.71	0.55
1:B:100:LEU:HD21	1:B:165:PHE:HD2	1.71	0.55
1:B:310:ALA:N	1:B:352:GLU:OE2	2.36	0.55
1:A:238:VAL:HB	1:A:241:HIS:O	2.06	0.55
1:B:216:LEU:HB2	1:B:229:GLU:HG3	1.88	0.55
1:A:103:GLU:HA	1:A:103:GLU:OE1	2.07	0.55
1:A:139:MET:HE2	1:A:140:ASP:HB2	1.89	0.55
1:A:207:LEU:O	1:A:226:ASN:HB3	2.07	0.55
1:A:120:VAL:HG13	1:A:121:ARG:H	1.72	0.54
1:A:185:HIS:CD2	1:A:187:HIS:ND1	2.75	0.54
1:A:290:ALA:O	1:A:294:ILE:HG13	2.07	0.54
1:B:287:TYR:HE2	1:B:329:ARG:HB3	1.73	0.54
1:A:151:SER:HA	5:B:608:HCZ:H13	1.90	0.54
1:B:73:LYS:CG	1:B:289:PRO:HD2	2.37	0.54
4:A:405:DXC:C21	4:B:602:DXC:H151	2.38	0.54
1:B:185:HIS:CD2	1:B:187:HIS:ND1	2.74	0.54
1:A:142:LEU:CD2	1:A:144:PHE:CD2	2.80	0.54
1:B:259:LEU:HD21	4:B:607:DXC:H72	1.89	0.53
1:A:120:VAL:HG21	1:A:139:MET:CA	2.38	0.53
1:A:290:ALA:HA	1:A:293:GLU:CG	2.38	0.53
1:A:194:ASN:HA	1:A:197:ILE:HG12	1.90	0.53
1:A:101:ASP:HA	1:A:166:ARG:NH2	2.21	0.53
1:A:285:THR:HG21	1:A:291:PHE:CZ	2.44	0.53
1:B:88:LYS:HD3	1:B:348:ALA:O	2.07	0.53
1:A:62:ASP:CA	1:A:232:TRP:HE1	2.21	0.53
1:B:287:TYR:CD1	1:B:288:CYS:N	2.73	0.53
1:A:233:TRP:CE3	1:A:233:TRP:HA	2.43	0.53
1:B:232:TRP:CE3	1:B:232:TRP:HA	2.44	0.53
1:A:142:LEU:HD22	1:A:144:PHE:CD2	2.38	0.53
1:A:175:LEU:HB3	1:A:178:ILE:HD11	1.91	0.53
1:B:183:ILE:HD12	1:B:191:LEU:HD13	1.90	0.53
1:B:280:PHE:O	1:B:304:ALA:HA	2.09	0.52
1:B:130:LEU:HA	1:B:169:PRO:HG2	1.90	0.52
1:B:308:ILE:HG12	1:B:341:ALA:HB1	1.90	0.52
1:A:347:PHE:HB2	1:A:349:LEU:CD1	2.39	0.52
1:A:314:ARG:HD3	1:A:318:LYS:HE2	1.91	0.52
1:B:343:HIS:O	1:B:344:TRP:CD1	2.63	0.52
1:A:86:MET:HA	1:A:86:MET:HE2	1.90	0.52
1:A:77:ILE:CG1	1:A:78:PRO:CD	2.88	0.52
1:A:140:ASP:OD2	1:A:276:TRP:N	2.30	0.52
1:A:175:LEU:O	1:A:202:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLU:OE1	1:A:206:GLU:N	2.32	0.52
1:B:313:PRO:HD2	1:B:351:ASN:HB2	1.92	0.52
1:B:67:ASN:H	1:B:68:PRO:CD	2.20	0.52
1:B:136:MET:HE2	1:B:143:ILE:CG2	2.40	0.51
1:A:280:PHE:HB2	1:A:301:PHE:CD2	2.45	0.51
1:A:77:ILE:HG12	1:A:78:PRO:HD2	1.93	0.51
3:A:403:3PE:H2A1	3:A:403:3PE:H3D2	1.91	0.51
1:B:185:HIS:CE1	1:B:284:ASP:HB2	2.46	0.51
1:B:256:LYS:NZ	1:B:258:THR:O	2.40	0.51
1:A:77:ILE:CG1	1:A:78:PRO:HD2	2.40	0.51
1:A:134:THR:HB	1:A:148:PRO:HA	1.92	0.51
1:A:353:HIS:HE1	1:A:355:LEU:HD12	1.76	0.51
1:B:175:LEU:O	1:B:202:ARG:NH1	2.43	0.51
4:A:406:DXC:C23	4:A:406:DXC:H161	2.41	0.51
1:B:214:GLY:N	1:B:229:GLU:OE2	2.36	0.51
1:B:123:ALA:HA	1:B:276:TRP:HE1	1.75	0.51
1:B:232:TRP:CZ2	1:B:250:PRO:HA	2.46	0.51
1:B:219:MET:HE2	1:B:219:MET:HA	1.93	0.50
1:B:71:THR:HG22	1:B:267:TRP:CZ2	2.46	0.50
1:B:97:LYS:HG3	1:B:167:ARG:HH22	1.75	0.50
1:A:92:SER:HB3	1:A:353:HIS:HA	1.93	0.50
1:A:83:TRP:CH2	1:A:162:PRO:HB3	2.46	0.50
1:B:308:ILE:HD12	1:B:357:PRO:CB	2.41	0.50
1:B:312:GLU:CG	1:B:351:ASN:HB3	2.40	0.50
1:B:312:GLU:HB3	1:B:351:ASN:H	1.77	0.50
1:A:196:VAL:HG13	1:A:209:TRP:CZ3	2.46	0.50
3:A:403:3PE:H3A1	4:B:601:DXC:H21	1.93	0.50
1:A:90:HIS:C	1:A:92:SER:N	2.69	0.50
1:B:187:HIS:CG	3:B:605:3PE:H12	2.47	0.50
1:B:216:LEU:O	1:B:220:GLN:HG3	2.11	0.50
1:A:231:ASP:O	1:A:234:GLU:HB2	2.12	0.50
1:A:314:ARG:CZ	1:A:318:LYS:HA	2.42	0.50
1:B:123:ALA:CA	1:B:276:TRP:HE1	2.25	0.50
1:B:125:LEU:HD23	1:B:139:MET:HB3	1.93	0.50
1:B:308:ILE:HD12	1:B:357:PRO:HB2	1.93	0.50
1:A:83:TRP:NE1	1:A:88:LYS:HA	2.24	0.49
1:A:204:GLY:N	1:A:206:GLU:OE1	2.46	0.49
1:A:313:PRO:HD3	1:A:351:ASN:HB2	1.95	0.49
1:B:84:LEU:O	1:B:85:ILE:HG13	2.11	0.49
1:A:130:LEU:HA	1:A:169:PRO:HG2	1.94	0.49
1:A:254:TRP:NE1	1:A:320:GLN:OE1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:THR:HG21	1:A:291:PHE:HZ	1.77	0.49
1:A:317:MET:HE1	3:A:403:3PE:C12	2.42	0.49
1:A:325:GLU:O	1:A:329:ARG:HG2	2.13	0.49
1:B:312:GLU:O	1:B:317:MET:HG3	2.12	0.49
1:A:104:LEU:O	1:A:166:ARG:NE	2.43	0.49
1:A:156:PRO:HD3	1:A:188:TYR:CE2	2.47	0.49
1:A:308:ILE:HD13	1:A:341:ALA:HB1	1.93	0.49
1:A:82:ARG:HD3	1:A:256:LYS:HE2	1.94	0.49
1:A:188:TYR:HD2	3:A:403:3PE:H342	1.76	0.49
1:A:314:ARG:HA	1:A:314:ARG:NE	2.26	0.49
1:A:82:ARG:HG3	4:A:409:DXC:H181	1.94	0.49
1:B:62:ASP:N	1:B:62:ASP:OD1	2.41	0.49
1:B:191:LEU:O	1:B:257:ARG:NH2	2.45	0.49
1:B:341:ALA:CB	1:B:377:VAL:HG12	2.43	0.49
1:A:232:TRP:O	1:A:233:TRP:HB2	2.13	0.48
1:B:97:LYS:HG3	1:B:167:ARG:NH2	2.29	0.48
1:A:92:SER:CB	1:A:353:HIS:HA	2.43	0.48
1:A:120:VAL:HG13	1:A:121:ARG:N	2.27	0.48
1:B:171:THR:OG1	1:B:174:GLU:HG3	2.13	0.48
1:B:258:THR:HB	4:B:602:DXC:H1	1.95	0.48
1:B:353:HIS:HB3	1:B:356:GLU:HB2	1.95	0.48
1:A:103:GLU:HB3	1:A:355:LEU:HD21	1.96	0.48
1:A:137:VAL:HB	1:A:144:PHE:CE1	2.48	0.48
1:A:349:LEU:HD12	1:A:349:LEU:N	2.28	0.48
1:B:138:GLU:HG2	1:B:143:ILE:HG23	1.95	0.48
1:B:312:GLU:O	1:B:314:ARG:N	2.46	0.48
1:A:160:MET:HB3	1:A:160:MET:HE2	1.70	0.48
1:A:253:HIS:CG	1:A:254:TRP:H	2.32	0.48
1:A:280:PHE:CE1	1:A:294:ILE:HD13	2.48	0.48
3:B:605:3PE:H271	3:B:605:3PE:H2A2	1.49	0.48
1:A:67:ASN:CG	1:A:68:PRO:HD3	2.39	0.47
1:A:172:ILE:HD12	1:A:199:LEU:HD22	1.96	0.47
1:A:77:ILE:HG13	1:A:78:PRO:CD	2.45	0.47
1:A:312:GLU:O	1:A:350:ALA:HB1	2.15	0.47
1:B:127:VAL:HG21	1:B:340:MET:CE	2.42	0.47
1:B:216:LEU:HB2	1:B:229:GLU:CG	2.44	0.47
1:A:138:GLU:HB3	1:A:143:ILE:HD13	1.95	0.47
1:B:232:TRP:HA	1:B:232:TRP:HE3	1.80	0.47
1:A:151:SER:HG	1:A:192:ASP:CG	2.21	0.47
1:B:116[B]:GLU:OE1	1:B:117:GLU:N	2.45	0.47
1:B:254:TRP:CD1	1:B:254:TRP:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLY:HA2	1:A:300:PRO:C	2.40	0.47
1:A:363:GLU:O	1:A:366:GLU:HG3	2.13	0.47
1:B:312:GLU:HB3	1:B:313:PRO:HD2	1.97	0.47
1:A:131:GLY:O	1:A:132:HIS:C	2.58	0.47
1:A:243:LYS:HD2	1:A:243:LYS:N	2.29	0.47
1:A:187:HIS:CG	3:A:403:3PE:H12	2.50	0.47
1:A:313:PRO:HB3	1:A:315[B]:TRP:CZ3	2.50	0.47
1:B:210:PHE:HB3	1:B:270:TRP:CH2	2.50	0.47
1:A:246:PHE:CD2	1:A:272:VAL:HG22	2.50	0.46
1:B:153:ARG:HG2	1:B:155:SER:HB3	1.97	0.46
1:B:247:VAL:HG12	1:B:249:THR:HG23	1.97	0.46
1:A:123:ALA:HB1	1:A:276:TRP:CE3	2.50	0.46
1:A:178:ILE:HD12	1:A:203:PHE:HE2	1.80	0.46
1:B:160:MET:HE2	1:B:160:MET:HB3	1.75	0.46
1:B:172:ILE:HA	1:B:175:LEU:CD2	2.45	0.46
1:A:313:PRO:O	1:A:317:MET:HG2	2.15	0.46
1:B:105:PRO:HG2	1:B:379:LYS:HD2	1.97	0.46
1:B:259:LEU:CD2	4:B:607:DXC:H72	2.44	0.46
1:A:238:VAL:CG1	1:A:239:PRO:HD2	2.45	0.46
1:B:100:LEU:HD11	1:B:165:PHE:HB2	1.96	0.46
1:B:188:TYR:HE1	1:B:257:ARG:NH1	2.12	0.46
1:B:287:TYR:CE2	1:B:329:ARG:HB3	2.51	0.46
1:A:155:SER:HB2	1:A:161:GLY:HA3	1.97	0.46
1:A:311:TYR:O	1:A:317:MET:HB2	2.16	0.46
1:A:343:HIS:O	1:A:344:TRP:CD1	2.68	0.46
1:A:387:ASN:OD1	1:A:387:ASN:N	2.44	0.46
1:A:114:ASN:O	1:A:117:GLU:HG3	2.16	0.46
1:B:57:SER:C	1:B:59:LYS:H	2.23	0.46
1:B:92:SER:HB3	1:B:354:TYR:H	1.80	0.46
1:A:77:ILE:CD1	1:A:319:TYR:CE1	2.99	0.46
1:A:140:ASP:OD1	1:A:276:TRP:HB2	2.15	0.46
1:B:368:TYR:CD1	1:B:368:TYR:N	2.84	0.46
1:A:142:LEU:CD1	1:A:238:VAL:HG21	2.45	0.46
1:A:215:LEU:O	1:A:219:MET:HG2	2.16	0.46
1:B:311:TYR:HB3	1:B:322:VAL:O	2.16	0.46
1:B:312:GLU:CG	1:B:351:ASN:CB	2.94	0.45
3:B:605:3PE:H111	3:B:605:3PE:H31	1.99	0.45
1:A:106:VAL:HG21	1:A:167[B]:ARG:HH21	1.81	0.45
1:A:303:LEU:HD11	1:A:340:MET:HB2	1.98	0.45
1:B:125:LEU:HD22	1:B:139:MET:HB3	1.97	0.45
1:A:172:ILE:O	1:A:175:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:HIS:O	1:A:93:VAL:N	2.48	0.45
1:B:219:MET:HB3	1:B:227:VAL:HG11	1.98	0.45
1:A:145:LEU:O	1:A:181:VAL:HA	2.16	0.45
1:A:208:ARG:HD3	1:A:210:PHE:CZ	2.51	0.45
1:B:88:LYS:HG3	1:B:89:ASP:N	2.31	0.45
1:A:142:LEU:HD12	1:A:238:VAL:HG21	1.97	0.45
1:A:147:ASP:OD2	1:A:190:HIS:ND1	2.46	0.45
1:A:191:LEU:HD23	1:A:257:ARG:NH1	2.31	0.45
1:A:218:TRP:CD1	4:A:404:DXC:H3	2.52	0.45
1:A:296:LYS:N	1:A:296:LYS:HD2	2.31	0.45
1:A:361:LEU:HD21	1:A:375:PHE:CD1	2.52	0.45
1:A:228:ILE:HG21	1:A:236:ASN:ND2	2.32	0.45
4:A:404:DXC:H243	1:B:160:MET:HE1	1.99	0.45
1:A:136:MET:HA	1:A:145:LEU:HD23	1.98	0.45
1:A:233:TRP:HA	1:A:233:TRP:HE3	1.81	0.45
4:A:409:DXC:H221	4:A:409:DXC:H243	1.58	0.45
1:B:109:PRO:HG2	1:B:170:CYS:HB3	1.98	0.45
1:A:232:TRP:HZ3	1:A:267:TRP:CD1	2.35	0.44
1:A:314:ARG:NH2	1:A:321:HIS:O	2.44	0.44
1:B:59:LYS:HE2	1:B:59:LYS:HB2	1.47	0.44
1:A:231:ASP:OD1	1:A:232:TRP:N	2.50	0.44
1:A:120:VAL:HG22	1:A:121:ARG:N	2.33	0.44
1:B:137:VAL:HB	1:B:144:PHE:CE1	2.53	0.44
1:A:77:ILE:CG2	1:A:319:TYR:HB2	2.48	0.44
1:A:98:GLU:HG2	1:A:99:GLU:H	1.83	0.44
1:A:120:VAL:HG22	1:A:121:ARG:H	1.83	0.44
1:A:120:VAL:C	1:A:122:GLU:N	2.74	0.44
1:A:172:ILE:O	1:A:202:ARG:NH1	2.50	0.44
1:A:254:TRP:CD1	1:A:254:TRP:N	2.85	0.44
1:B:123:ALA:N	1:B:276:TRP:NE1	2.65	0.44
1:B:389:ASP:C	1:B:389:ASP:OD1	2.61	0.44
1:A:185:HIS:CD2	1:A:253:HIS:CD2	3.05	0.44
1:A:185:HIS:CD2	1:A:253:HIS:HD2	2.36	0.44
1:A:340:MET:O	1:A:341:ALA:HB3	2.18	0.44
1:B:192:ASP:O	1:B:196:VAL:HG23	2.17	0.43
1:A:132:HIS:HB3	1:A:133:ALA:H	1.61	0.43
1:A:219:MET:HB3	1:A:227:VAL:HG11	2.00	0.43
1:A:173:SER:HB2	1:B:97:LYS:HD2	1.99	0.43
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.77	0.43
1:A:78:PRO:O	1:A:79:ASN:C	2.62	0.43
1:A:126:ARG:HB3	1:A:138:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:TYR:HA	1:B:193:TYR:CE2	2.54	0.43
1:A:306:ILE:HG12	1:A:330:ILE:HG21	2.00	0.43
1:A:314:ARG:O	1:A:316:PHE:N	2.52	0.43
1:B:229:GLU:O	1:B:230:LEU:HD23	2.19	0.43
1:A:90:HIS:O	1:A:90:HIS:CG	2.71	0.43
1:B:205:ASN:OD1	1:B:225:GLU:HB2	2.19	0.43
1:A:296:LYS:HA	1:A:296:LYS:NZ	2.34	0.43
1:A:201:GLU:C	1:A:201:GLU:OE1	2.62	0.43
1:A:353:HIS:CE1	1:A:355:LEU:HD12	2.53	0.43
1:A:119:GLY:O	1:A:120:VAL:C	2.62	0.42
1:A:120:VAL:C	1:A:122:GLU:H	2.27	0.42
1:A:228:ILE:HD12	1:A:236:ASN:ND2	2.33	0.42
1:B:136:MET:HE1	1:B:176:PRO:CG	2.42	0.42
1:A:209:TRP:HB2	1:A:227:VAL:HG12	2.01	0.42
1:A:218:TRP:NE1	4:A:404:DXC:H3	2.34	0.42
1:A:259:LEU:HB2	4:A:406:DXC:O2	2.19	0.42
1:A:77:ILE:HG22	1:A:319:TYR:CB	2.48	0.42
1:A:365:LEU:HD12	1:A:365:LEU:HA	1.72	0.42
1:B:207:LEU:O	1:B:226:ASN:HB3	2.19	0.42
1:A:185:HIS:CE1	1:A:284:ASP:HB2	2.55	0.42
1:A:296:LYS:O	1:A:297:ARG:C	2.61	0.42
1:B:235:GLU:HB3	1:B:247:VAL:CG2	2.47	0.42
1:B:341:ALA:HB3	1:B:377:VAL:HG12	2.01	0.42
1:A:175:LEU:HD22	1:A:176:PRO:HD2	2.01	0.42
4:A:404:DXC:H203	1:B:159:TYR:HB3	2.01	0.42
1:A:96:SER:HB2	1:A:99:GLU:HB2	2.02	0.42
1:B:314:ARG:NH2	1:B:318:LYS:HB2	2.35	0.42
1:B:317:MET:O	1:B:318:LYS:C	2.62	0.42
1:A:81:LEU:CD2	1:A:86:MET:HB2	2.50	0.42
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.78	0.42
1:B:64:ARG:HG3	1:B:68:PRO:O	2.20	0.42
1:B:227:VAL:C	1:B:228:ILE:HD13	2.44	0.42
1:B:368:TYR:N	1:B:368:TYR:HD1	2.18	0.42
1:B:177:PRO:HA	1:B:203:PHE:HE2	1.85	0.42
1:B:215:LEU:O	1:B:219:MET:HG2	2.20	0.42
4:A:404:DXC:C20	1:B:159:TYR:HB3	2.50	0.41
1:B:69:TRP:CH2	1:B:213:LEU:HD23	2.55	0.41
1:B:82:ARG:HG2	4:B:607:DXC:H1	2.01	0.41
1:A:77:ILE:HG21	1:A:319:TYR:CG	2.55	0.41
1:A:330:ILE:HD13	1:A:330:ILE:HA	1.83	0.41
4:A:405:DXC:H161	4:A:405:DXC:H212	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASP:HA	1:B:63:GLY:HA3	1.67	0.41
1:A:59:LYS:HE2	1:A:297:ARG:HB2	2.01	0.41
1:A:142:LEU:HD21	1:A:144:PHE:HB3	2.02	0.41
4:A:408:DXC:H222	4:A:408:DXC:H243	1.79	0.41
1:B:230:LEU:HD13	1:B:234:GLU:O	2.19	0.41
1:A:90:HIS:O	1:A:92:SER:N	2.53	0.41
1:B:330:ILE:O	1:B:334:VAL:HG23	2.20	0.41
4:A:407:DXC:H1	3:B:605:3PE:H2D2	2.02	0.41
1:B:208:ARG:NH2	1:B:228:ILE:HD11	2.36	0.41
3:A:403:3PE:H232	3:A:403:3PE:H341	2.02	0.41
1:B:285:THR:HG21	1:B:291:PHE:CZ	2.56	0.41
1:B:364:ALA:O	1:B:367:ARG:HB2	2.20	0.41
1:A:139:MET:HE3	1:A:139:MET:HB2	1.81	0.41
1:B:71:THR:OG1	1:B:76[B]:SER:OG	2.33	0.41
1:B:120:VAL:HG13	1:B:122:GLU:N	2.36	0.41
1:A:384:ARG:HG2	1:A:386:LEU:CD2	2.50	0.41
1:A:96:SER:HB2	1:A:99:GLU:OE1	2.21	0.41
1:A:290:ALA:HA	1:A:293:GLU:CD	2.46	0.41
1:A:312:GLU:HG3	1:A:313:PRO:N	2.36	0.41
4:A:405:DXC:H61	4:A:408:DXC:H243	2.02	0.41
1:B:94:PRO:HA	1:B:354:TYR:CE1	2.56	0.41
1:B:142:LEU:CD1	1:B:244:VAL:HG11	2.50	0.41
1:B:191:LEU:HB3	1:B:257:ARG:HH21	1.86	0.41
1:B:215:LEU:HD22	1:B:218:TRP:HB3	2.03	0.41
1:B:340:MET:HE3	1:B:340:MET:HB3	1.64	0.41
1:A:156:PRO:HB3	1:A:188:TYR:OH	2.21	0.41
1:A:212:PRO:O	1:A:229:GLU:HG2	2.20	0.41
1:B:285:THR:O	1:B:322:VAL:HG13	2.21	0.41
1:B:153:ARG:CG	1:B:155:SER:HB3	2.51	0.40
1:A:77:ILE:CG2	1:A:319:TYR:CB	2.99	0.40
1:A:324:PRO:O	1:A:328:VAL:HG23	2.21	0.40
1:B:232:TRP:CZ3	1:B:250:PRO:HA	2.56	0.40
1:A:120:VAL:CG1	1:A:121:ARG:HH21	2.34	0.40
1:B:241:HIS:ND1	1:B:241:HIS:N	2.69	0.40
1:A:236:ASN:CG	1:A:237:CYS:H	2.22	0.40
4:A:404:DXC:H181	4:A:407:DXC:C23	2.50	0.40
1:B:92:SER:HB3	1:B:354:TYR:HD1	1.85	0.40
3:B:605:3PE:H281	3:B:605:3PE:H3B2	2.03	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	333/393 (85%)	274 (82%)	47 (14%)	12 (4%)	2	5
1	B	335/393 (85%)	296 (88%)	30 (9%)	9 (3%)	4	9
All	All	668/786 (85%)	570 (85%)	77 (12%)	21 (3%)	3	7

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	A	119	GLY
1	B	66	VAL
1	B	85	ILE
1	B	312	GLU
1	B	313	PRO
1	A	58	LYS
1	A	91	SER
1	A	120	VAL
1	A	315[A]	TRP
1	A	315[B]	TRP
1	A	79	ASN
1	B	57	SER
1	B	89	ASP
1	A	59	LYS
1	B	67	ASN
1	B	95	SER
1	A	344	TRP
1	B	344	TRP
1	A	67	ASN
1	A	313	PRO

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%)	270 (91%)	28 (9%)	8	18
1	B	299/352 (85%)	278 (93%)	21 (7%)	14	29
All	All	597/704 (85%)	548 (92%)	49 (8%)	10	23

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	59	LYS
1	A	61	LYS
1	A	62	ASP
1	A	67	ASN
1	A	80	VAL
1	A	81	LEU
1	A	82	ARG
1	A	88	LYS
1	A	90	HIS
1	A	121	ARG
1	A	122	GLU
1	A	125	LEU
1	A	132	HIS
1	A	134	THR
1	A	135	VAL
1	A	143	ILE
1	A	155	SER
1	A	230	LEU
1	A	241	HIS
1	A	296	LYS
1	A	312	GLU
1	A	314	ARG
1	A	320	GLN
1	A	343	HIS
1	A	344	TRP
1	A	365	LEU

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Mol	Chain	Res	Type
1	A	387	ASN
1	B	59	LYS
1	B	66	VAL
1	B	67	ASN
1	B	85	ILE
1	B	88	LYS
1	B	93	VAL
1	B	97	LYS
1	B	100	LEU
1	B	126	ARG
1	B	157	SER
1	B	172	ILE
1	B	199	LEU
1	B	232	TRP
1	B	288	CYS
1	B	313	PRO
1	B	314	ARG
1	B	317	MET
1	B	329	ARG
1	B	334	VAL
1	B	343	HIS
1	B	355	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	220	GLN
1	A	252	GLN
1	A	277	ASN
1	A	351	ASN
1	A	362	ASN
1	B	67	ASN

5.3.3 RNA ⓘ

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 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	$\# Z > 2$
3	3PE	B	605	2	43,43,50	0.52	0	46,48,55	0.90	1 (2%)
3	3PE	A	403	2	43,43,50	0.55	0	46,48,55	0.82	1 (2%)
4	DXC	A	409	-	31,31,31	0.57	0	49,49,49	1.14	6 (12%)
4	DXC	B	606	-	31,31,31	0.68	0	49,49,49	1.25	4 (8%)
4	DXC	A	407	-	31,31,31	0.63	0	49,49,49	1.21	5 (10%)
4	DXC	A	404	-	31,31,31	0.71	0	49,49,49	1.22	4 (8%)
4	DXC	A	406	-	31,31,31	0.69	0	49,49,49	1.22	2 (4%)
4	DXC	A	405	-	31,31,31	0.60	0	49,49,49	1.02	2 (4%)
4	DXC	B	601	-	31,31,31	0.65	1 (3%)	49,49,49	0.86	1 (2%)
5	HCZ	B	608	-	18,18,18	1.38	2 (11%)	29,29,29	1.26	3 (10%)
4	DXC	B	607	-	31,31,31	0.64	0	49,49,49	1.09	4 (8%)
4	DXC	A	408	-	31,31,31	0.55	0	49,49,49	1.05	2 (4%)
4	DXC	B	602	-	31,31,31	0.65	0	49,49,49	1.48	8 (16%)

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	3PE	B	605	2	-	23/47/47/54	-
3	3PE	A	403	2	-	24/47/47/54	-
4	DXC	A	409	-	-	6/9/71/71	0/4/4/4
4	DXC	B	606	-	-	3/9/71/71	0/4/4/4
4	DXC	A	407	-	-	0/9/71/71	0/4/4/4
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	A	405	-	-	4/9/71/71	0/4/4/4
4	DXC	B	601	-	-	0/9/71/71	0/4/4/4
5	HCZ	B	608	-	-	6/6/19/19	0/2/2/2
4	DXC	B	607	-	-	8/9/71/71	0/4/4/4
4	DXC	A	408	-	-	8/9/71/71	0/4/4/4
4	DXC	B	602	-	-	5/9/71/71	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	608	HCZ	S02-N01	2.69	1.65	1.60
5	B	608	HCZ	S15-N14	2.48	1.66	1.63
4	B	601	DXC	C22-C23	2.15	1.55	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	DXC	C12-C11-C9	-4.24	110.13	114.69
4	B	602	DXC	C11-C9-C10	-4.15	103.66	109.09
4	B	602	DXC	C8-C9-C10	3.58	114.81	110.52
4	B	602	DXC	C15-C11-C12	3.43	106.87	103.54
4	B	606	DXC	C12-C17-C19	3.40	123.61	119.48
4	A	406	DXC	C14-C10-C4	3.35	117.10	113.70
4	A	406	DXC	C16-C15-C11	-3.18	98.91	105.14
3	B	605	3PE	O12-P-O14	3.04	126.59	112.44
4	B	606	DXC	C21-C19-C17	-2.90	104.31	110.33
5	B	608	HCZ	C05-S02-N01	-2.82	103.21	108.28
4	A	404	DXC	O1-C13-C14	2.81	114.83	109.12
4	A	404	DXC	C11-C12-C13	2.79	109.97	107.42
3	A	403	3PE	O12-P-O14	2.67	124.85	112.44
4	A	404	DXC	O1-C13-C12	-2.64	106.56	111.02
5	B	608	HCZ	O03-S02-N01	2.56	111.04	107.35
4	A	409	DXC	C4-C10-C9	2.54	115.01	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	DXC	C14-C13-C12	2.52	113.82	111.26
4	A	409	DXC	C10-C14-C13	-2.49	111.03	114.29
4	A	407	DXC	C12-C17-C19	2.48	122.49	119.48
4	A	409	DXC	C16-C17-C12	-2.46	101.15	103.54
4	A	407	DXC	C2-C3-C4	2.45	115.27	112.66
4	B	607	DXC	C4-C10-C9	2.44	114.91	112.43
4	B	601	DXC	C20-C12-C17	-2.42	107.41	111.20
4	A	407	DXC	C3-C2-C1	2.42	116.35	112.71
4	A	408	DXC	C18-C4-C5	-2.37	104.54	108.31
4	A	407	DXC	C10-C4-C3	2.29	111.70	108.51
4	B	606	DXC	C18-C4-C5	-2.28	104.68	108.31
4	B	607	DXC	C16-C15-C11	-2.24	100.76	105.14
5	B	608	HCZ	O16-S15-N14	-2.23	105.86	107.92
4	B	606	DXC	C22-C21-C19	2.20	118.57	114.46
4	A	405	DXC	O1-C13-C14	2.18	113.55	109.12
4	A	409	DXC	C14-C13-C12	-2.15	109.08	111.26
4	B	607	DXC	O1-C13-C12	-2.13	107.42	111.02
4	A	404	DXC	C14-C10-C4	-2.13	111.55	113.70
4	B	602	DXC	C4-C10-C9	2.12	114.58	112.43
4	A	407	DXC	C20-C12-C11	-2.11	107.90	111.20
4	B	602	DXC	C10-C14-C13	2.11	117.05	114.29
4	A	405	DXC	O1-C13-C12	-2.09	107.48	111.02
4	B	607	DXC	C18-C4-C5	-2.08	104.99	108.31
4	A	409	DXC	C17-C12-C13	2.04	119.50	117.67
4	B	602	DXC	C18-C4-C5	-2.01	105.10	108.31
4	A	409	DXC	C20-C12-C13	-2.01	107.04	109.06
4	A	408	DXC	C16-C17-C19	2.01	115.23	112.18

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	3PE	C1-O11-P-O12
3	A	403	3PE	C1-O11-P-O13
3	A	403	3PE	C11-O13-P-O11
3	A	403	3PE	C11-O13-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	C11-O13-P-O12
3	B	605	3PE	O13-C11-C12-N
5	B	608	HCZ	C10-C05-S02-N01

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Mol	Chain	Res	Type	Atoms
5	B	608	HCZ	C10-C05-S02-O03
5	B	608	HCZ	C10-C05-S02-O04
4	A	408	DXC	C24-C19-C21-C22
4	A	409	DXC	C19-C21-C22-C23
3	A	403	3PE	O32-C31-O31-C3
3	B	605	3PE	O32-C31-O31-C3
3	A	403	3PE	C38-C39-C3A-C3B
3	B	605	3PE	C32-C31-O31-C3
4	A	405	DXC	C17-C19-C21-C22
3	A	403	3PE	C32-C31-O31-C3
3	B	605	3PE	C38-C39-C3A-C3B
4	B	607	DXC	C24-C19-C21-C22
4	A	404	DXC	C24-C19-C21-C22
4	A	409	DXC	C24-C19-C21-C22
4	A	406	DXC	C19-C21-C22-C23
4	A	408	DXC	C12-C17-C19-C21
4	A	406	DXC	C17-C19-C21-C22
3	B	605	3PE	C29-C2A-C2B-C2C
4	A	405	DXC	C24-C19-C21-C22
4	A	406	DXC	C24-C19-C21-C22
4	A	408	DXC	C12-C17-C19-C24
4	B	602	DXC	C19-C21-C22-C23
4	A	408	DXC	C17-C19-C21-C22
3	A	403	3PE	C21-C22-C23-C24
4	B	606	DXC	C24-C19-C21-C22
3	A	403	3PE	C29-C2A-C2B-C2C
4	A	408	DXC	C16-C17-C19-C24
5	B	608	HCZ	C06-C05-S02-O03
5	B	608	HCZ	C06-C05-S02-O04
5	B	608	HCZ	C06-C05-S02-N01
4	A	408	DXC	C16-C17-C19-C21
3	B	605	3PE	C37-C38-C39-C3A
3	B	605	3PE	C3A-C3B-C3C-C3D
3	A	403	3PE	C23-C24-C25-C26
4	B	602	DXC	C16-C17-C19-C24
3	A	403	3PE	C33-C34-C35-C36
3	B	605	3PE	C32-C33-C34-C35
3	A	403	3PE	C27-C28-C29-C2A
3	A	403	3PE	C2B-C2C-C2D-C2E
3	B	605	3PE	C2B-C2C-C2D-C2E
3	A	403	3PE	C32-C33-C34-C35
3	B	605	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
3	A	403	3PE	C3A-C3B-C3C-C3D
3	A	403	3PE	O11-C1-C2-O21
3	A	403	3PE	C36-C37-C38-C39
3	A	403	3PE	O11-C1-C2-C3
3	B	605	3PE	O11-C1-C2-C3
4	B	602	DXC	C12-C17-C19-C24
3	B	605	3PE	O11-C1-C2-O21
4	B	607	DXC	C19-C21-C22-C23
3	B	605	3PE	C36-C37-C38-C39
4	A	406	DXC	C12-C17-C19-C24
4	A	406	DXC	C12-C17-C19-C21
4	A	404	DXC	C12-C17-C19-C24
4	B	607	DXC	C12-C17-C19-C24
4	A	406	DXC	C16-C17-C19-C21
4	B	602	DXC	C16-C17-C19-C21
4	B	607	DXC	C16-C17-C19-C21
4	B	607	DXC	C12-C17-C19-C21
3	A	403	3PE	C1-O11-P-O14
3	A	403	3PE	C11-O13-P-O12
3	B	605	3PE	C1-O11-P-O14
3	B	605	3PE	C11-O13-P-O11
3	B	605	3PE	C11-O13-P-O14
4	B	607	DXC	C16-C17-C19-C24
4	B	602	DXC	C12-C17-C19-C21
4	A	406	DXC	C16-C17-C19-C24
4	A	406	DXC	C21-C22-C23-O4
4	A	409	DXC	C12-C17-C19-C24
4	B	607	DXC	C21-C22-C23-O3
4	A	406	DXC	C21-C22-C23-O3
4	B	607	DXC	C21-C22-C23-O4
4	A	408	DXC	C21-C22-C23-O4
4	A	404	DXC	C12-C17-C19-C21
4	A	408	DXC	C21-C22-C23-O3
3	B	605	3PE	C23-C24-C25-C26
4	A	404	DXC	C21-C22-C23-O3
3	A	403	3PE	C3C-C3D-C3E-C3F
4	A	409	DXC	C21-C22-C23-O4
3	A	403	3PE	O31-C31-C32-C33
4	A	404	DXC	C21-C22-C23-O4
4	A	405	DXC	C21-C22-C23-O4
4	A	409	DXC	C21-C22-C23-O3
3	B	605	3PE	O31-C31-C32-C33

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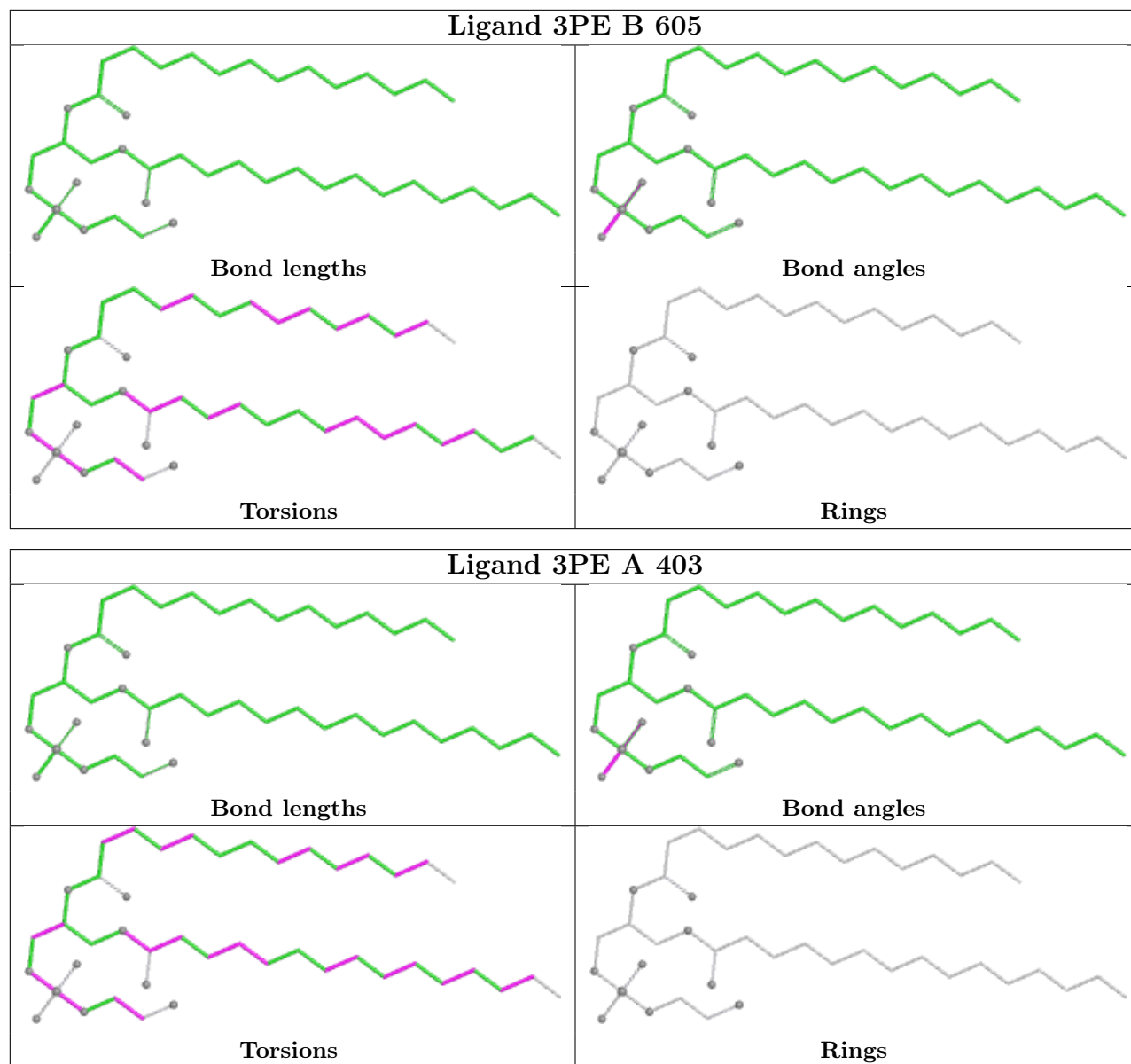
Mol	Chain	Res	Type	Atoms
4	B	606	DXC	C21-C22-C23-O4
3	B	605	3PE	C26-C27-C28-C29
4	A	405	DXC	C21-C22-C23-O3
4	A	409	DXC	C12-C17-C19-C21
4	B	606	DXC	C21-C22-C23-O3
3	A	403	3PE	O32-C31-C32-C33
3	B	605	3PE	O32-C31-C32-C33

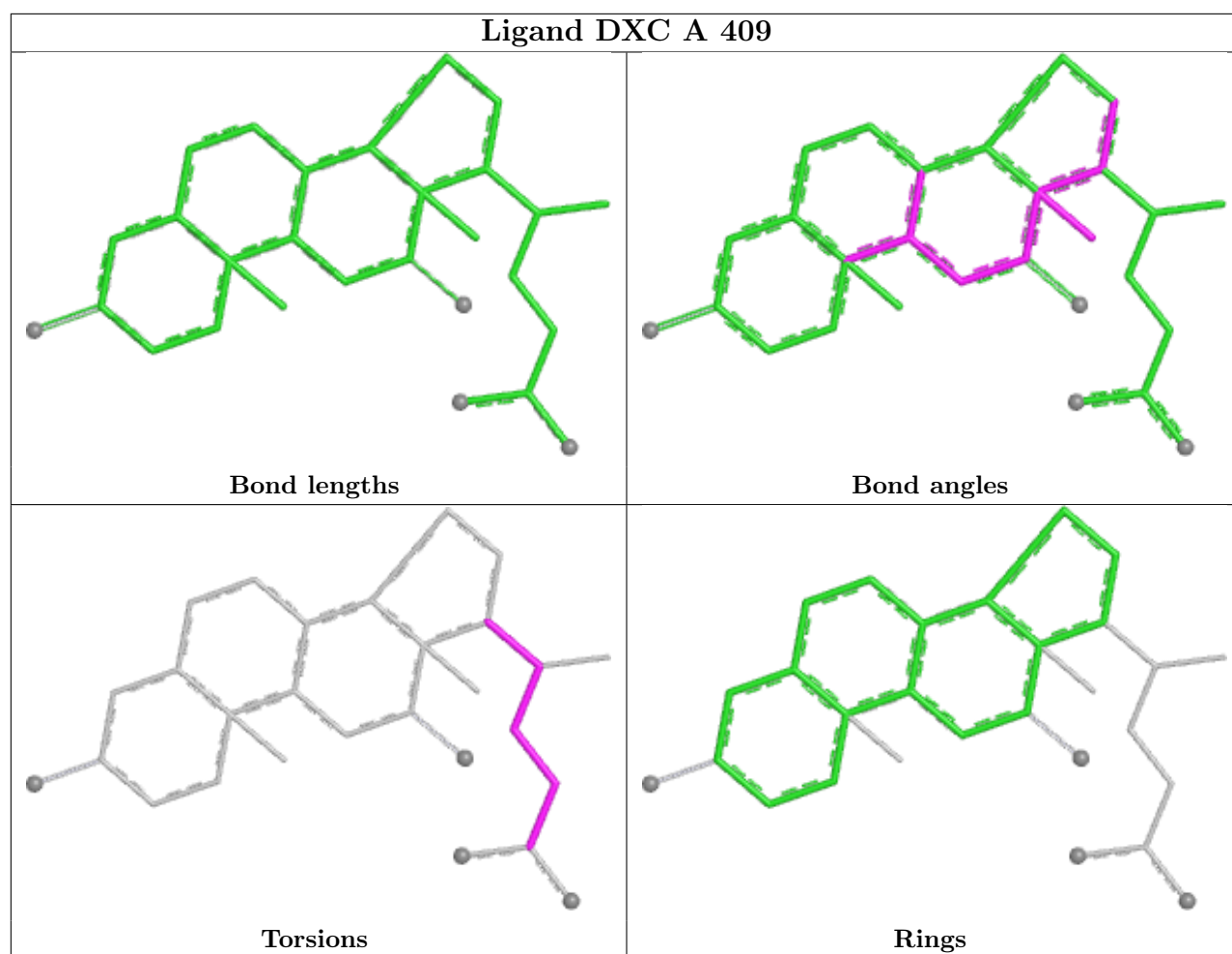
There are no ring outliers.

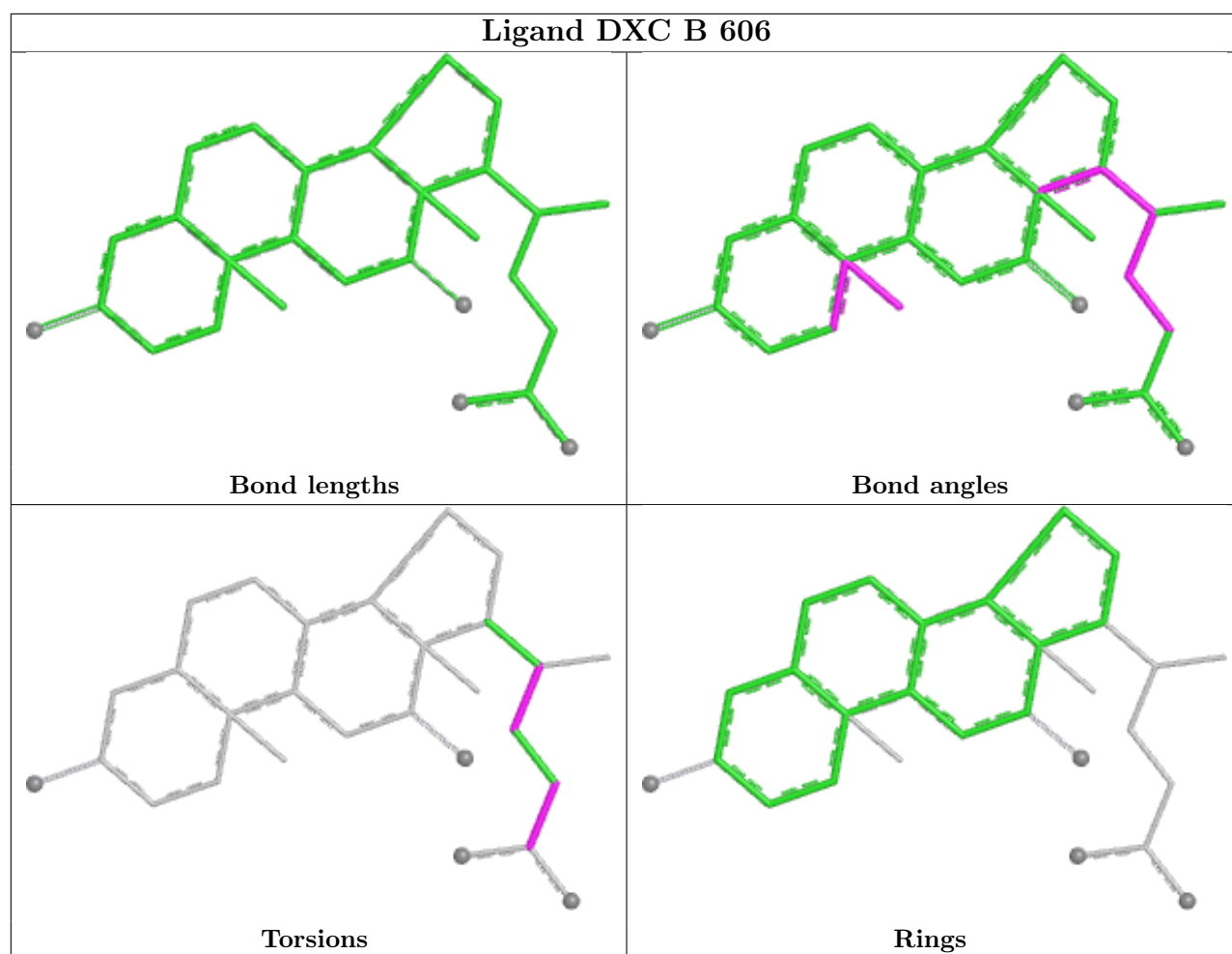
12 monomers are involved in 39 short contacts:

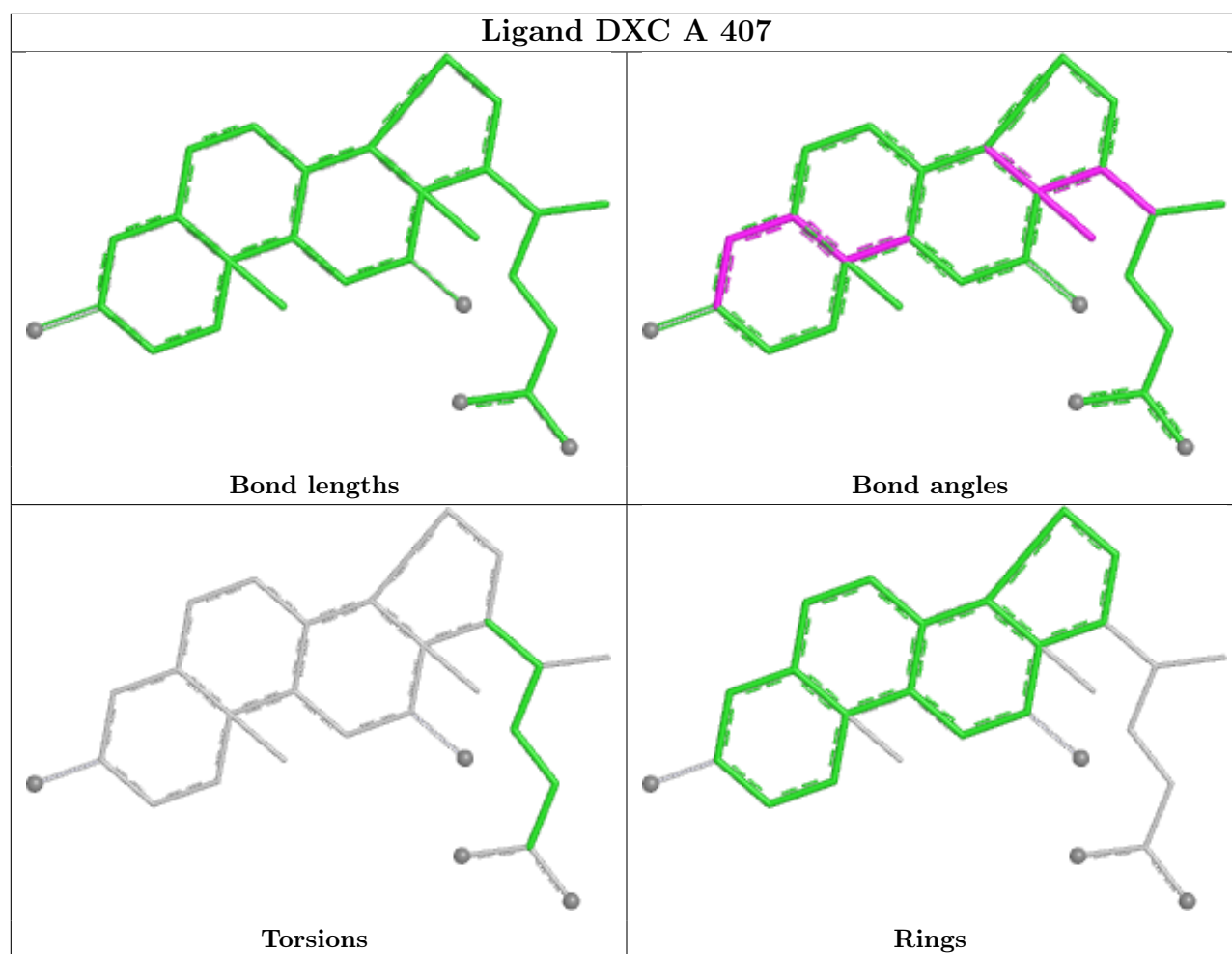
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	605	3PE	5	0
3	A	403	3PE	8	0
4	A	409	DXC	5	0
4	A	407	DXC	3	0
4	A	404	DXC	6	0
4	A	406	DXC	3	0
4	A	405	DXC	5	0
4	B	601	DXC	2	0
5	B	608	HCZ	1	0
4	B	607	DXC	3	0
4	A	408	DXC	2	0
4	B	602	DXC	5	0

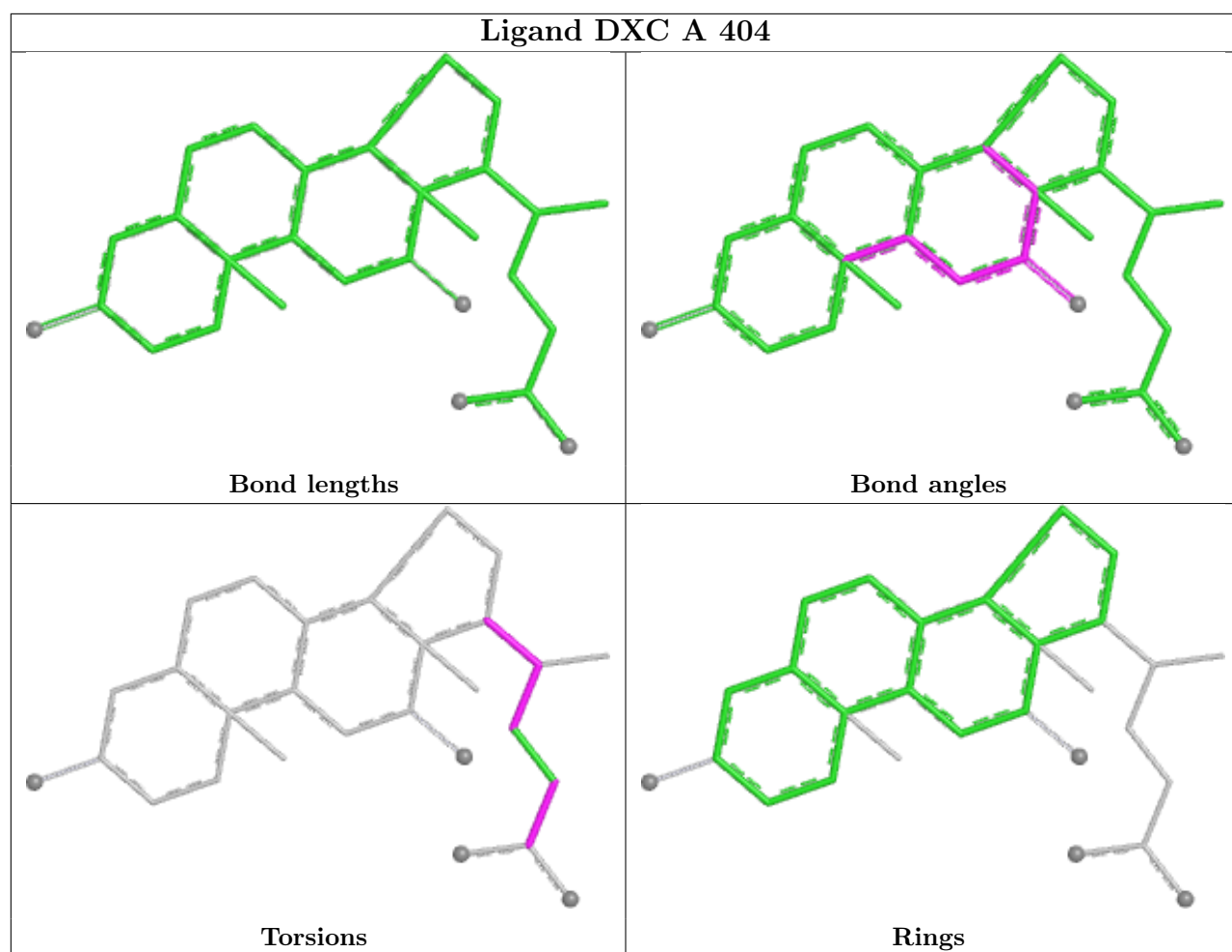
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

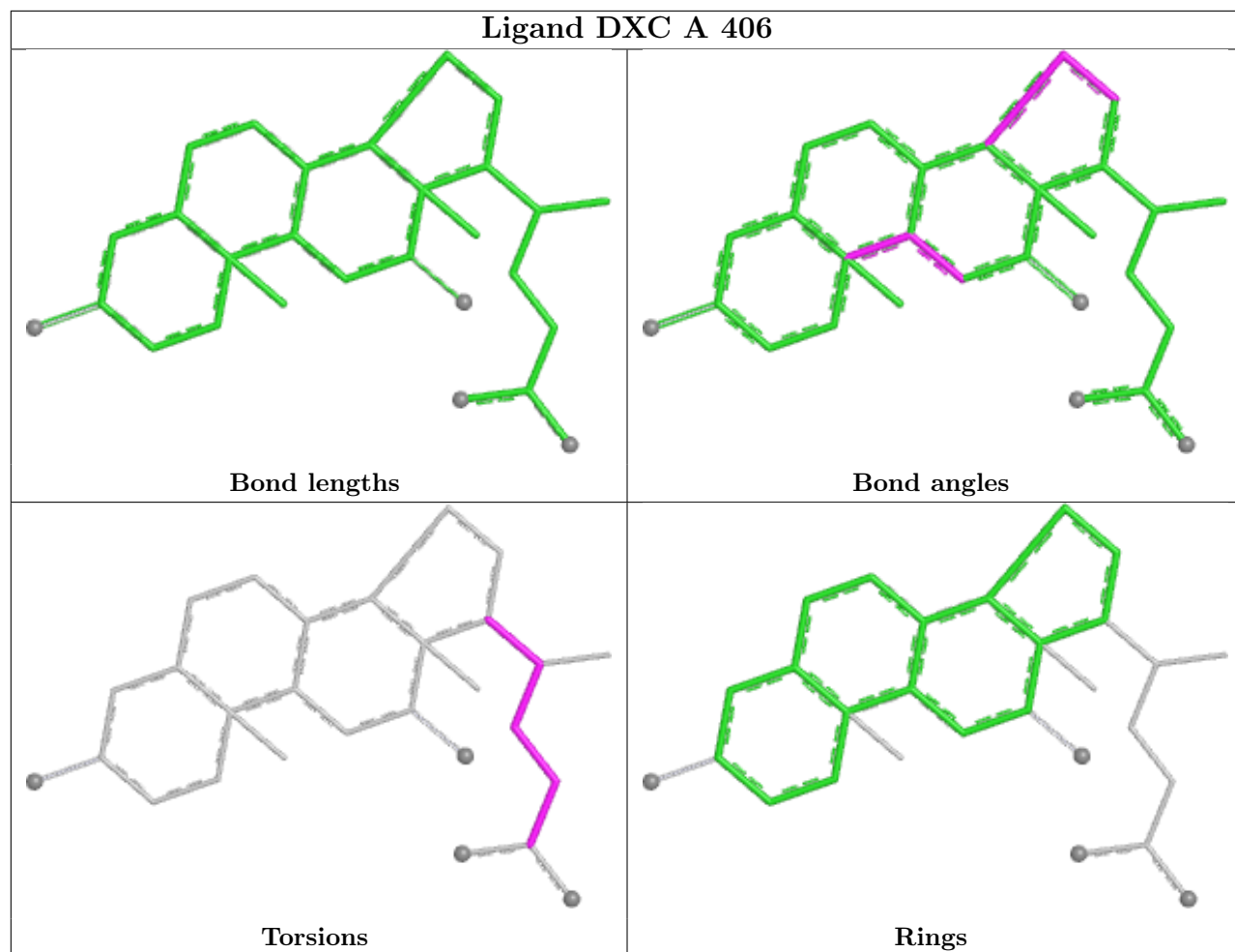


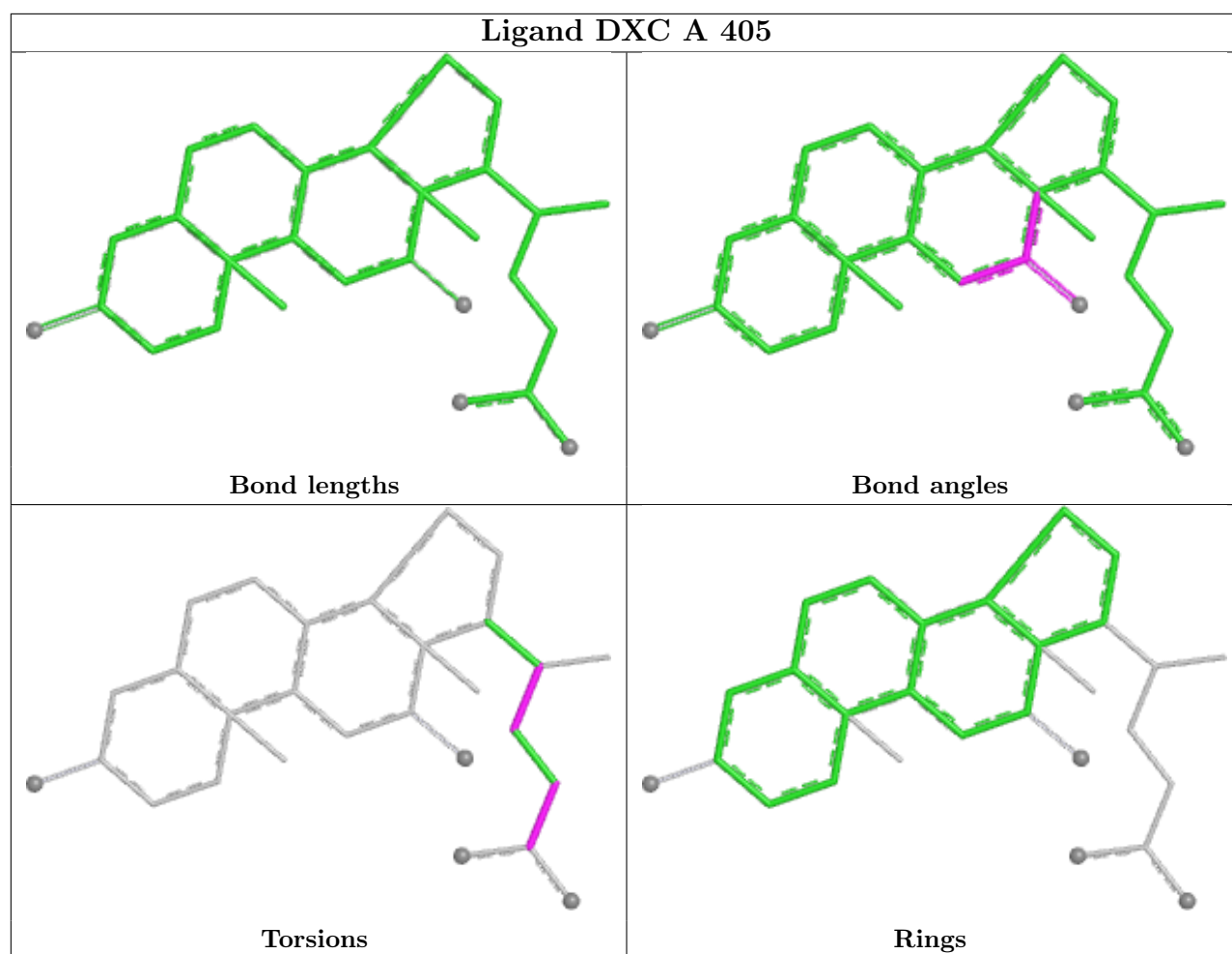


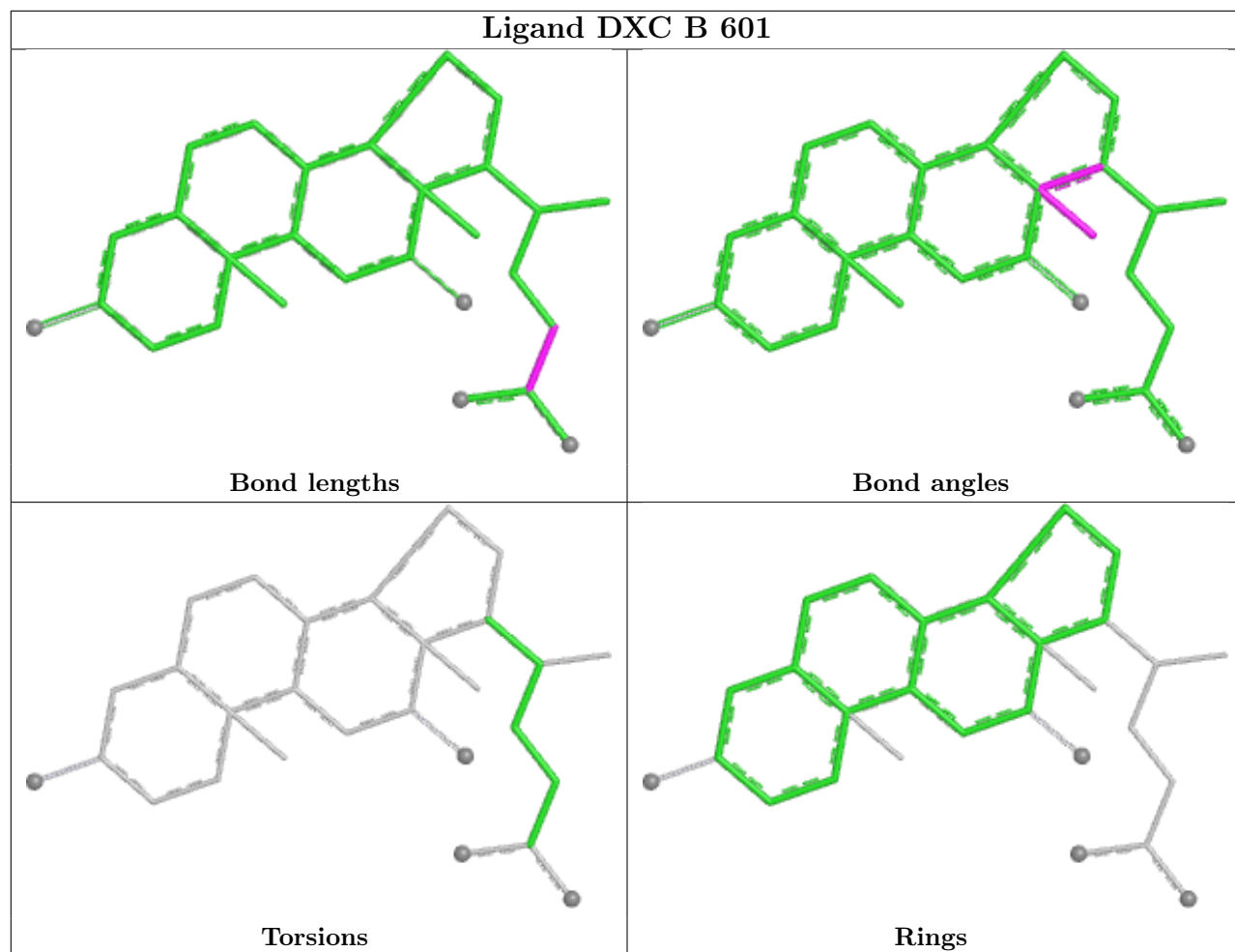


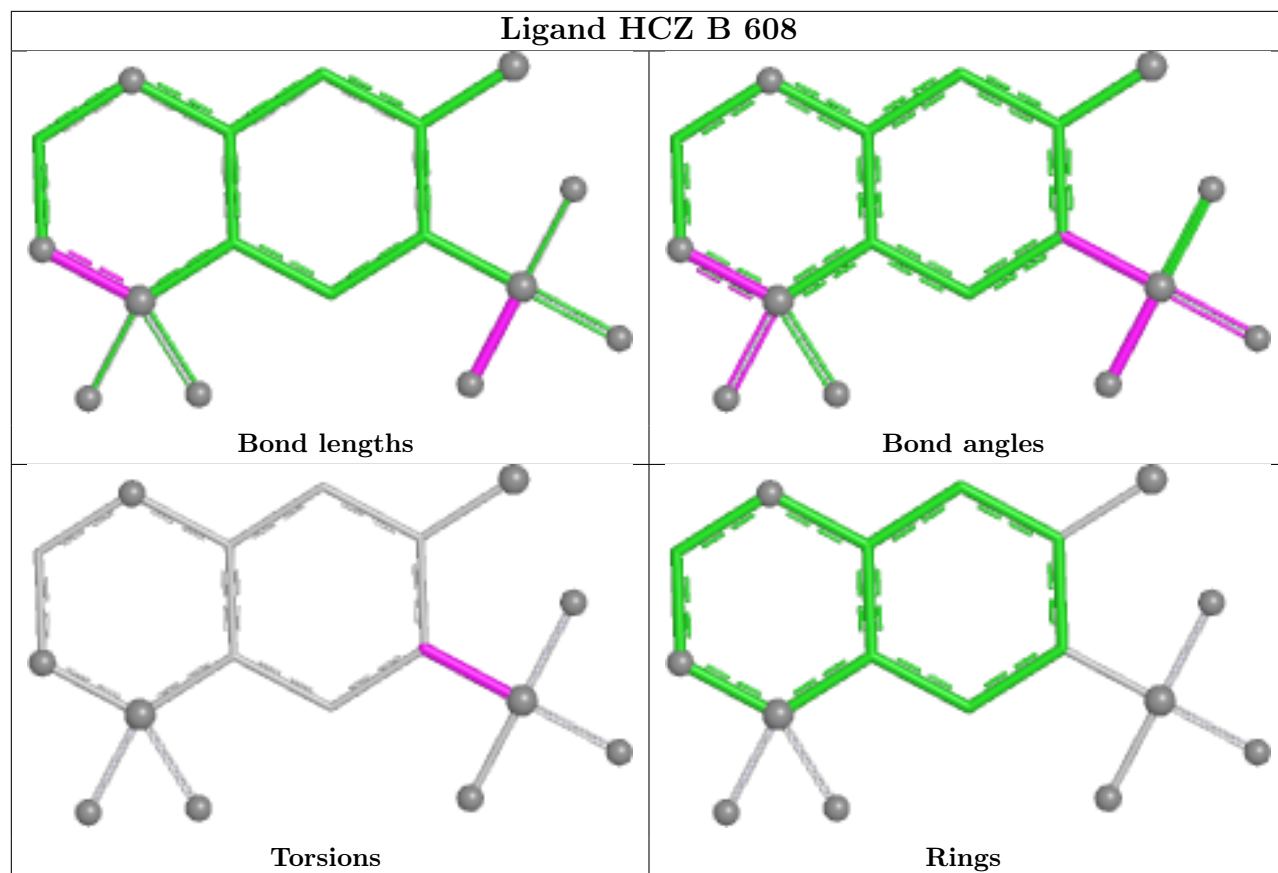


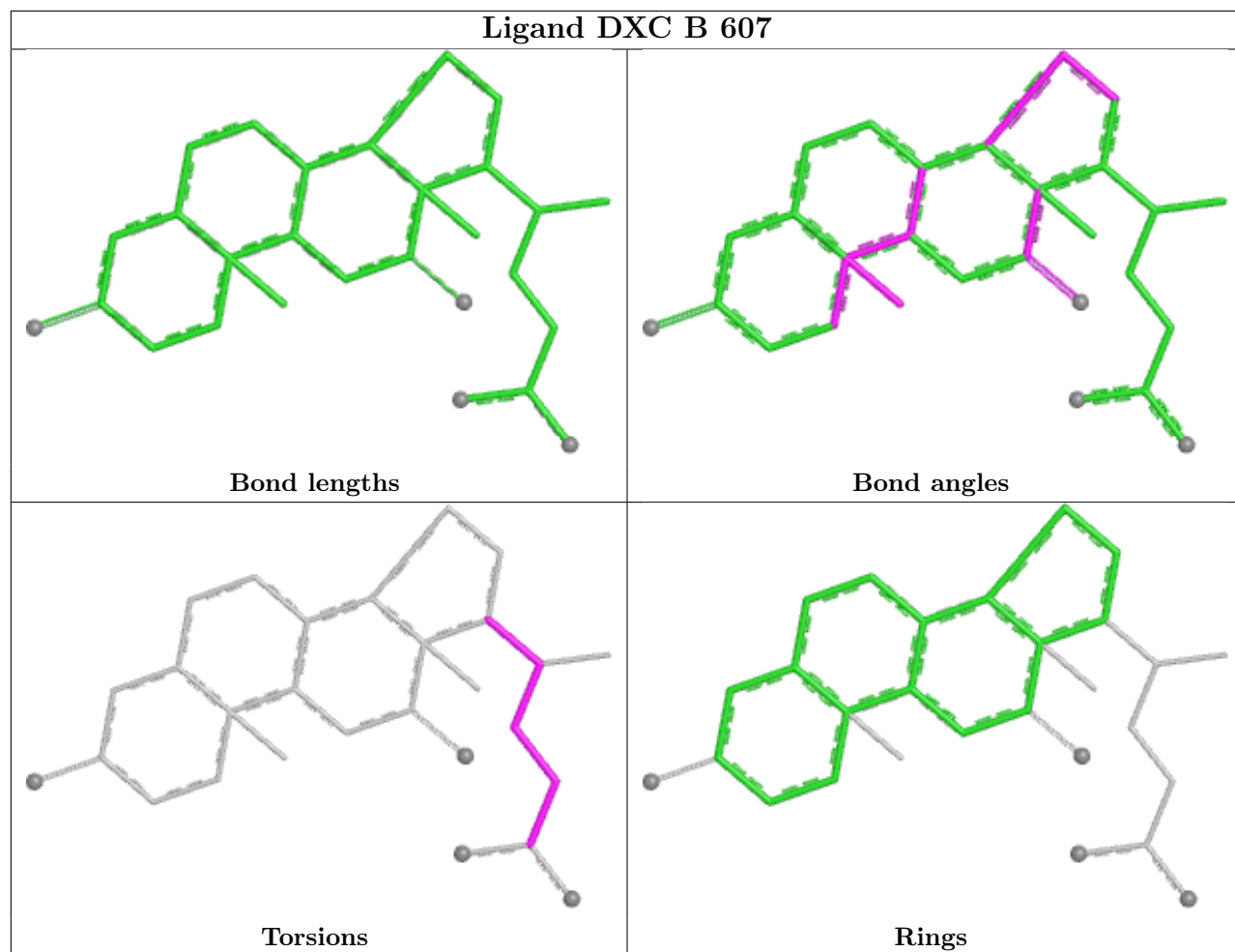


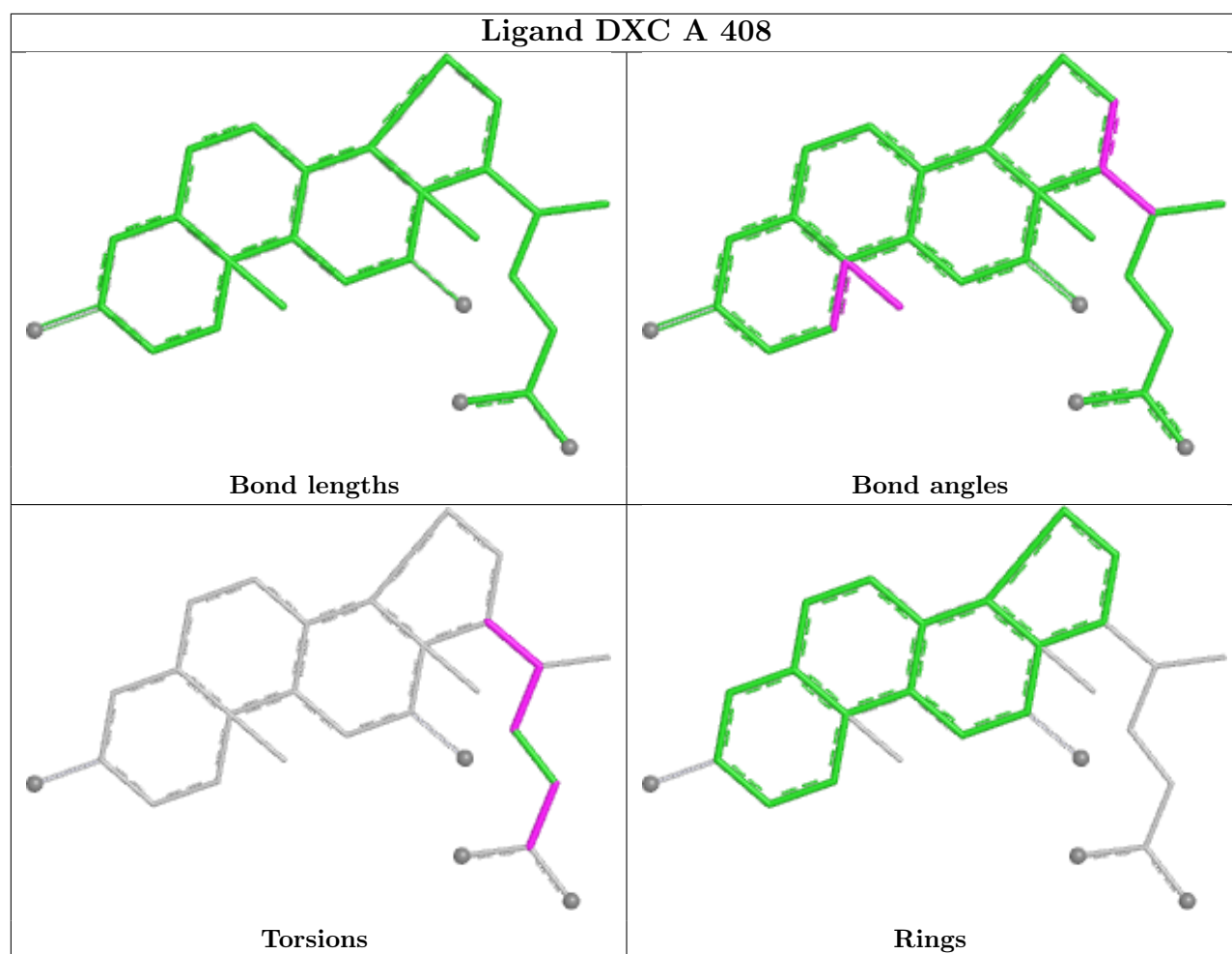


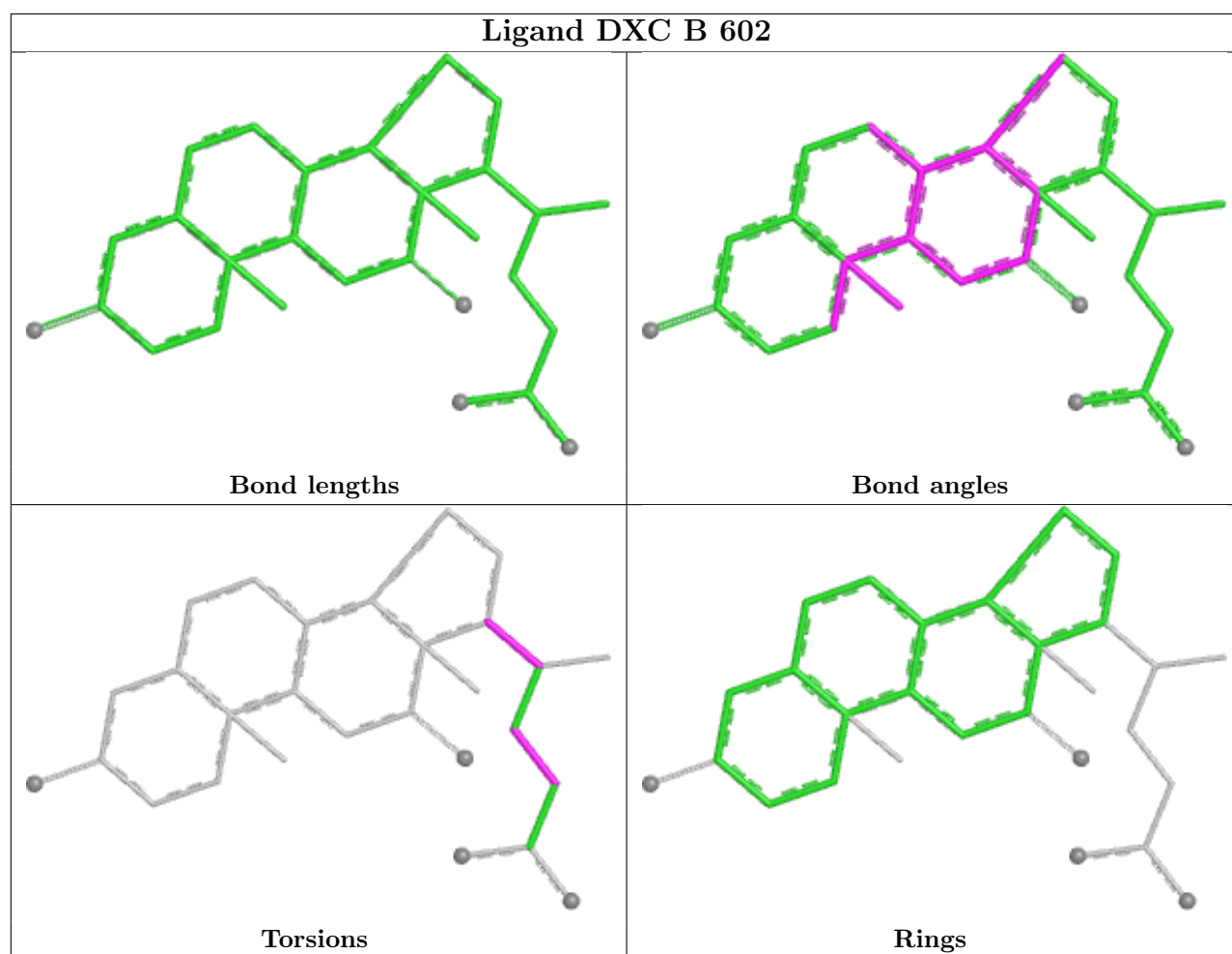












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	332/393 (84%)	0.73	40 (12%) 9 7	52, 104, 151, 183	3 (0%)
1	B	334/393 (84%)	0.56	35 (10%) 11 9	50, 86, 142, 174	3 (0%)
All	All	666/786 (84%)	0.65	75 (11%) 10 8	50, 96, 147, 183	6 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	84	LEU	7.6
1	A	84	LEU	5.7
1	B	72	TRP	5.2
1	B	85	ILE	5.2
1	B	66	VAL	4.8
1	A	72[A]	TRP	4.4
1	A	340	MET	4.4
1	A	85	ILE	4.4
1	A	142	LEU	4.3
1	A	63	GLY	4.0
1	A	82	ARG	3.9
1	B	297	ARG	3.9
1	A	83	TRP	3.9
1	A	60	GLY	3.8
1	A	167[A]	ARG	3.7
1	A	314	ARG	3.6
1	A	134	THR	3.4
1	B	233	TRP	3.4
1	B	80	VAL	3.3
1	B	77	ILE	3.3
1	B	100	LEU	3.3
1	A	69	TRP	3.3
1	B	83	TRP	3.3
1	B	71	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	87	GLU	3.2
1	B	296	LYS	3.0
1	B	87	GLU	3.0
1	B	93	VAL	3.0
1	A	66	VAL	2.9
1	A	80	VAL	2.9
1	B	65	PHE	2.9
1	A	71	THR	2.8
1	B	69	TRP	2.8
1	B	81	LEU	2.7
1	A	81	LEU	2.7
1	A	74	ASN	2.7
1	A	107	LEU	2.7
1	B	298	PHE	2.7
1	B	97	LYS	2.6
1	B	88	LYS	2.6
1	B	340	MET	2.6
1	A	244	VAL	2.5
1	A	363	GLU	2.5
1	A	118	ALA	2.5
1	A	93	VAL	2.5
1	B	73	LYS	2.5
1	B	98	GLU	2.4
1	B	86	MET	2.4
1	B	96	SER	2.4
1	A	298	PHE	2.3
1	A	59	LYS	2.3
1	A	273	LEU	2.3
1	A	73	LYS	2.3
1	A	77	ILE	2.3
1	A	94	PRO	2.3
1	A	287	TYR	2.3
1	B	59	LYS	2.2
1	B	367	ARG	2.2
1	A	70	PRO	2.2
1	B	120	VAL	2.2
1	B	368	TYR	2.2
1	B	123	ALA	2.2
1	A	78	PRO	2.2
1	A	319	TYR	2.2
1	A	294	ILE	2.1
1	B	68	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	88	LYS	2.1
1	B	175	LEU	2.1
1	A	62	ASP	2.1
1	B	232	TRP	2.1
1	A	90	HIS	2.0
1	A	135	VAL	2.0
1	A	388	ASN	2.0
1	B	92	SER	2.0
1	B	330	ILE	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.

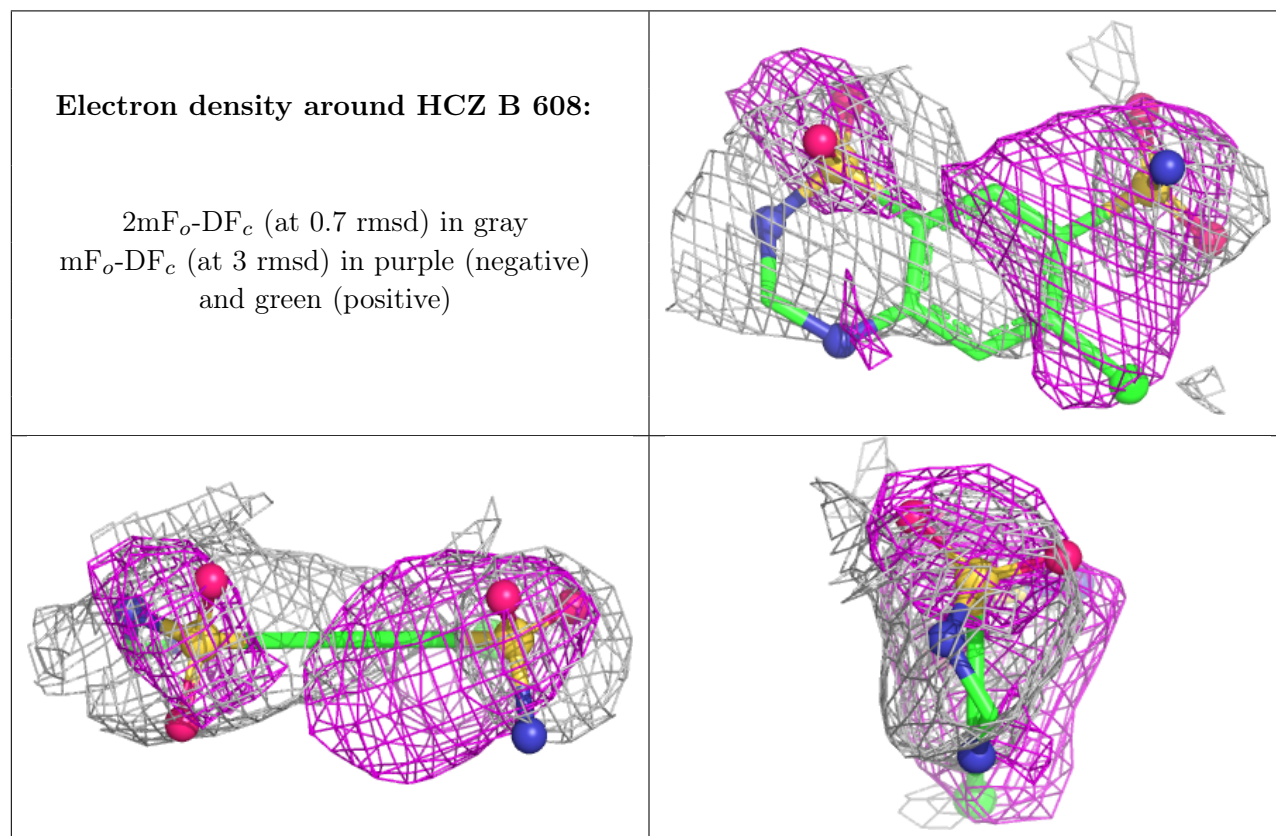
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	HCZ	B	608	17/17	0.54	0.16	109,126,141,146	0
4	DXC	A	409	28/28	0.79	0.22	129,138,157,159	0
4	DXC	B	607	28/28	0.82	0.24	114,118,130,137	0
4	DXC	A	406	28/28	0.88	0.17	92,98,102,103	28
4	DXC	B	606	28/28	0.90	0.16	86,91,105,113	0
4	DXC	A	404	28/28	0.90	0.14	81,85,99,102	0
4	DXC	B	602	28/28	0.90	0.15	83,88,92,96	28
4	DXC	A	405	28/28	0.91	0.15	87,94,100,106	0
4	DXC	A	407	28/28	0.93	0.15	77,81,84,86	0
4	DXC	A	408	28/28	0.94	0.12	74,79,92,101	0
3	3PE	A	403	44/51	0.94	0.15	82,90,95,98	0
3	3PE	B	605	44/51	0.95	0.15	80,89,95,96	0
4	DXC	B	601	28/28	0.95	0.15	77,83,86,87	0
2	ZN	B	603	1/1	0.99	0.07	82,82,82,82	0

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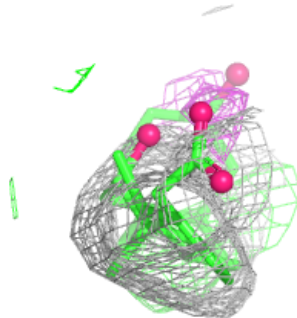
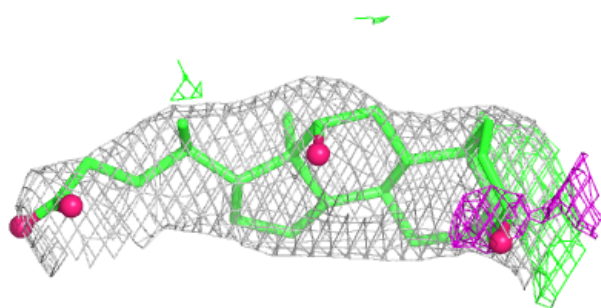
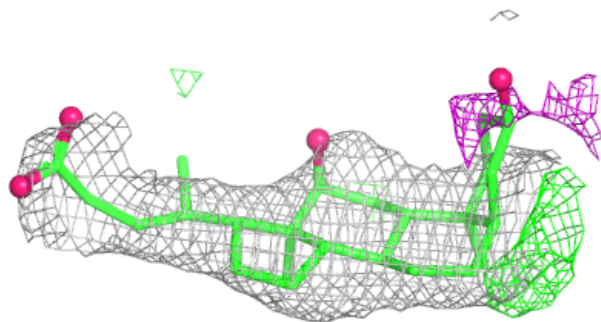
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	604	1/1	0.99	0.05	89,89,89,89	0
2	ZN	A	401	1/1	0.99	0.04	85,85,85,85	0
2	ZN	A	402	1/1	1.00	0.05	88,88,88,88	0

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.

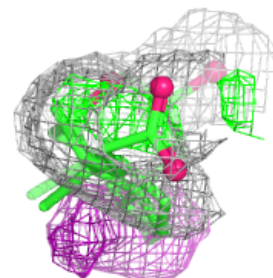
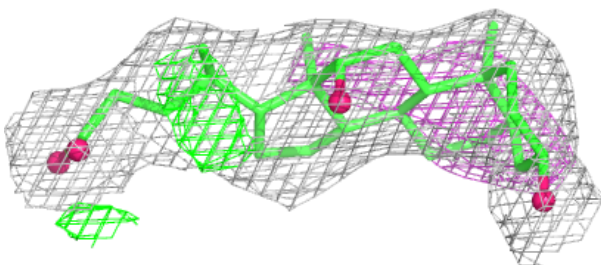
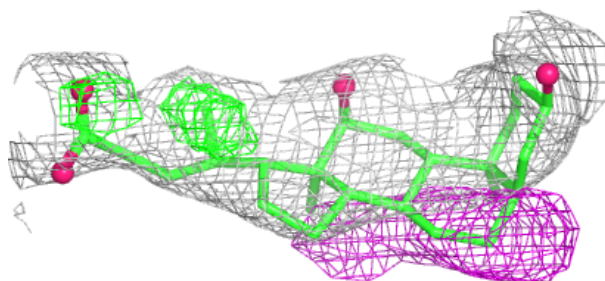


Electron density around DXC A 409:

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

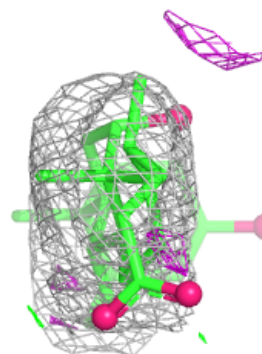
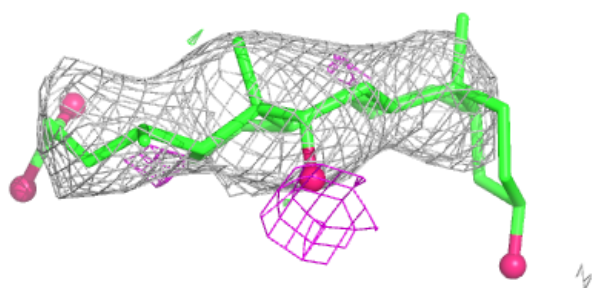
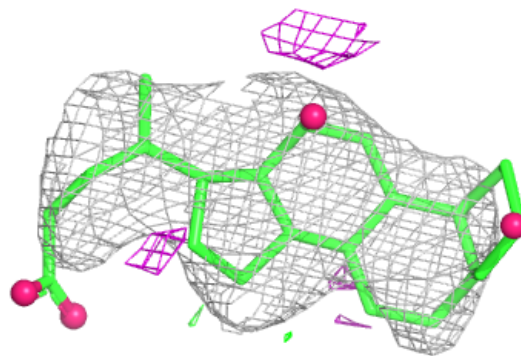
**Electron density around DXC B 607:**

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

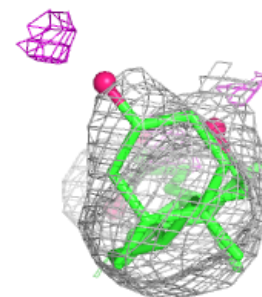
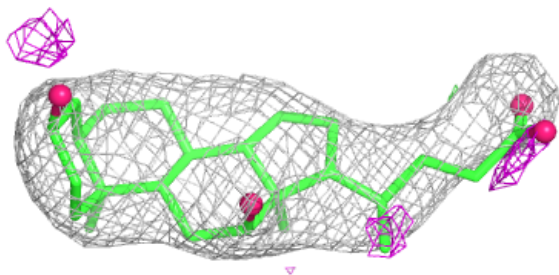
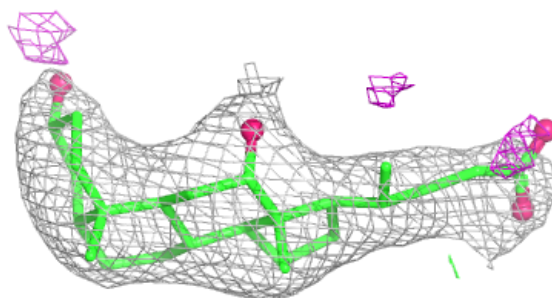


Electron density around DXC A 406:

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

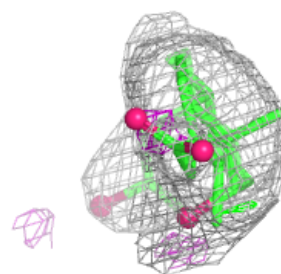
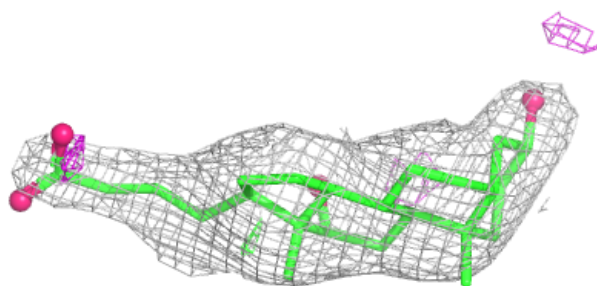
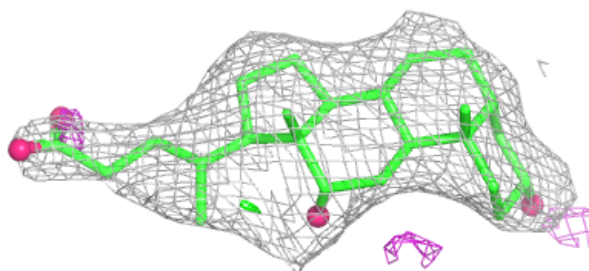
**Electron density around DXC B 606:**

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

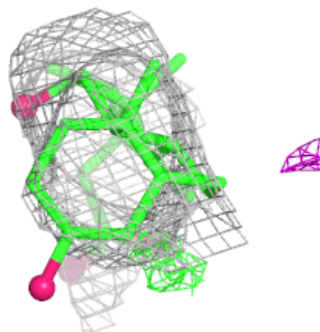
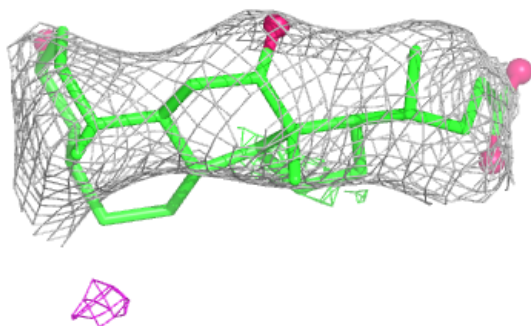
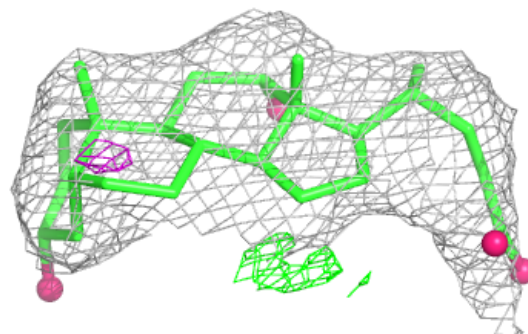


Electron density around DXC A 404:

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

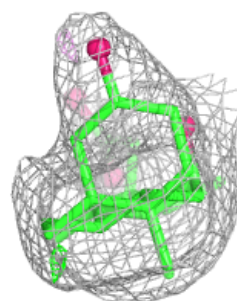
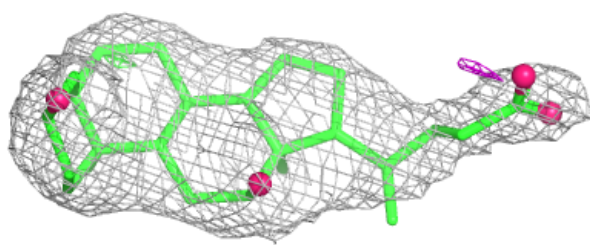
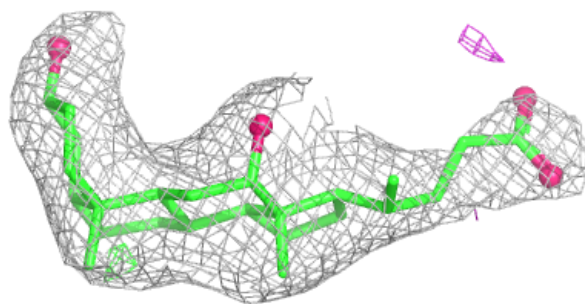
**Electron density around DXC B 602:**

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

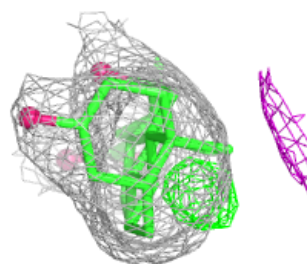
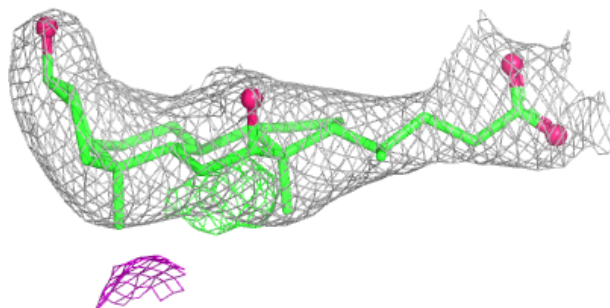
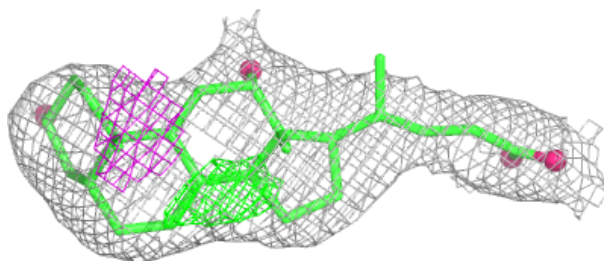


Electron density around DXC A 405:

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

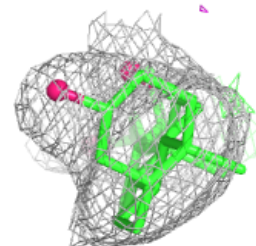
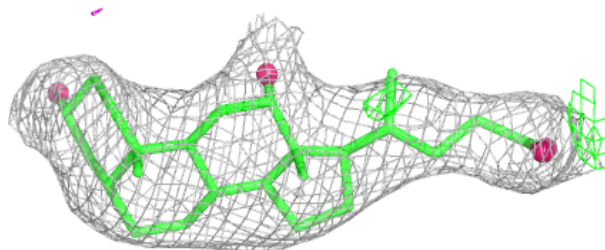
**Electron density around DXC A 407:**

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

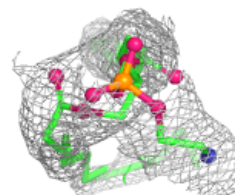
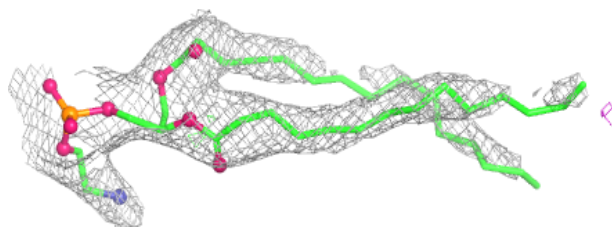
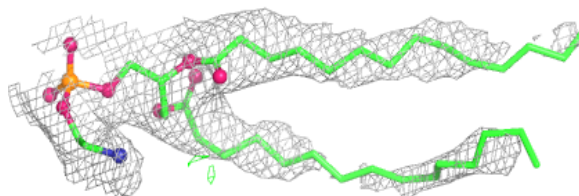


Electron density around DXC A 408:

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

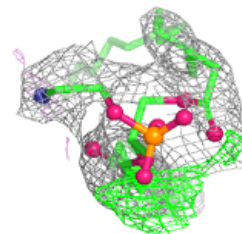
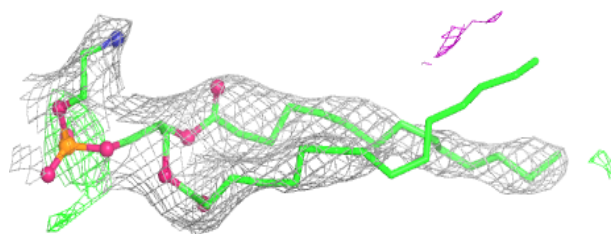
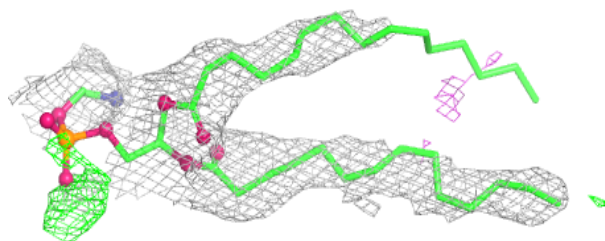
**Electron density around 3PE A 403:**

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

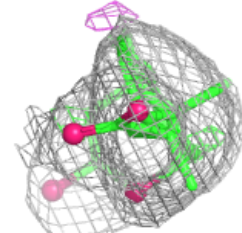
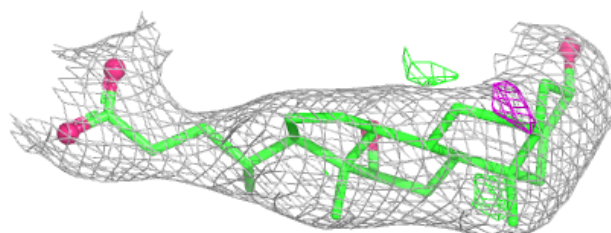
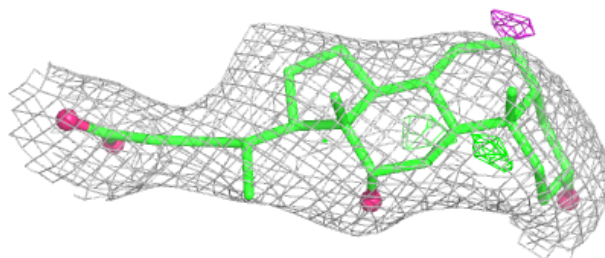


Electron density around 3PE B 605:

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

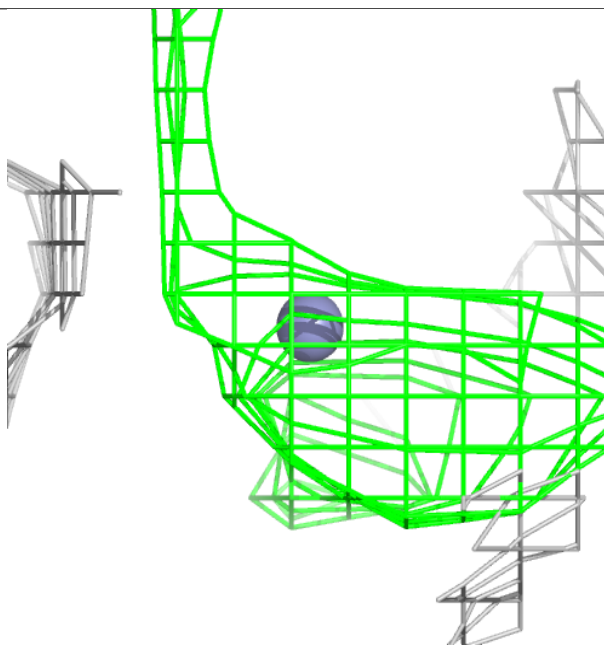
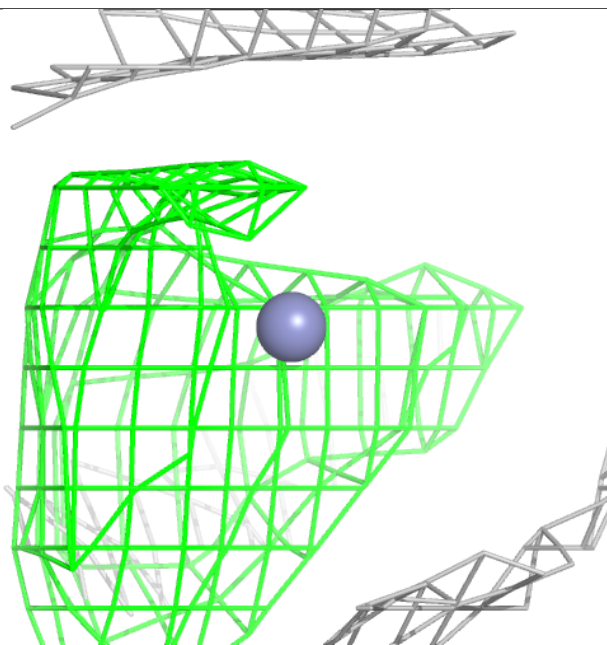
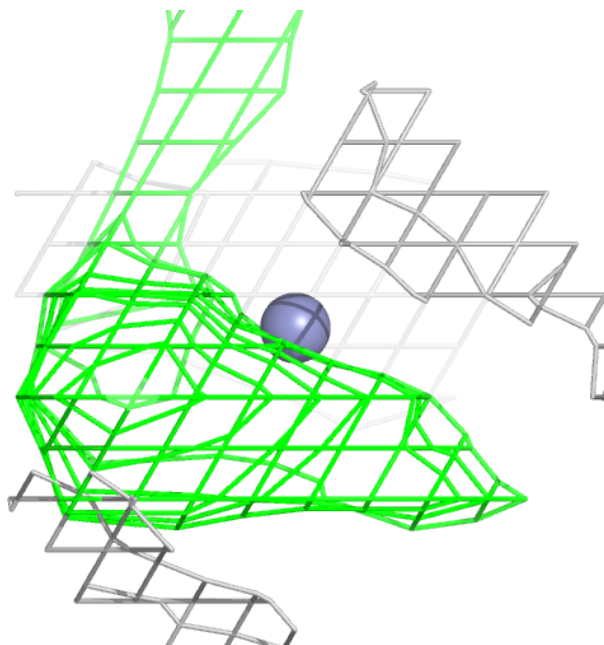
**Electron density around DXC B 601:**

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



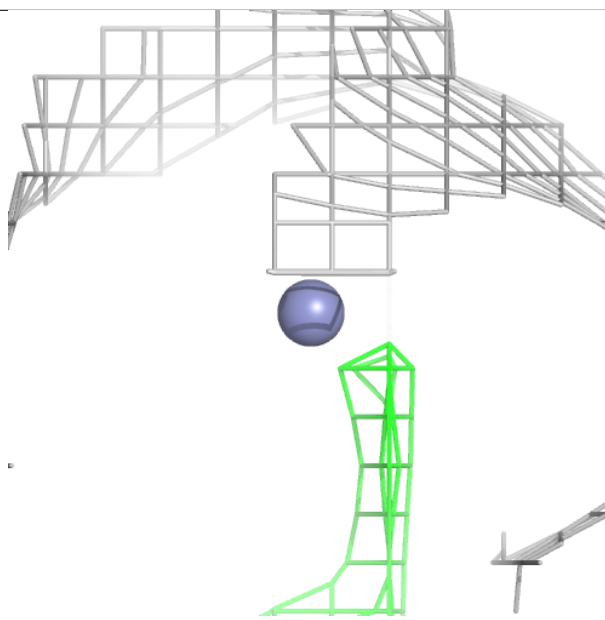
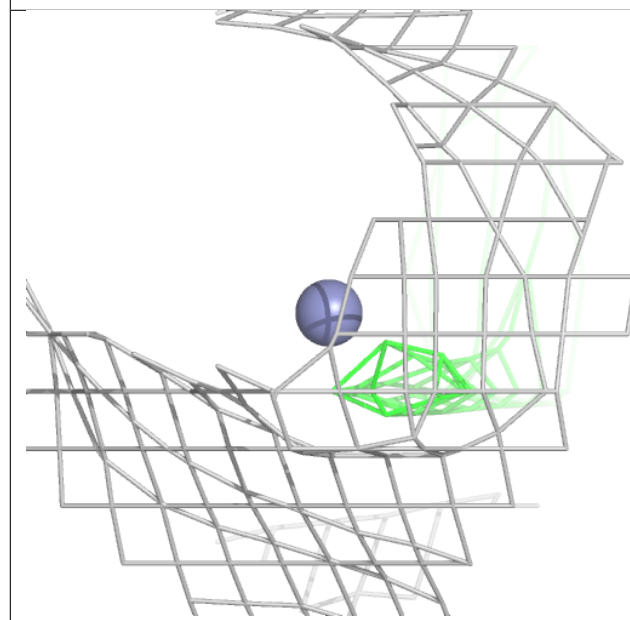
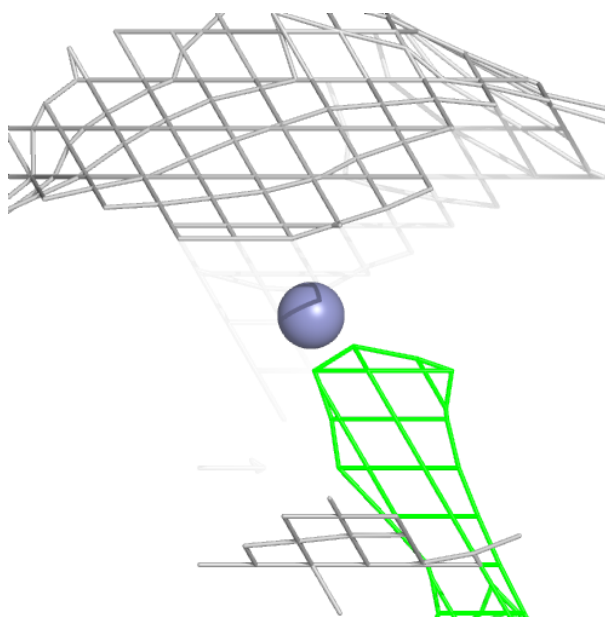
Electron density around ZN B 603:

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



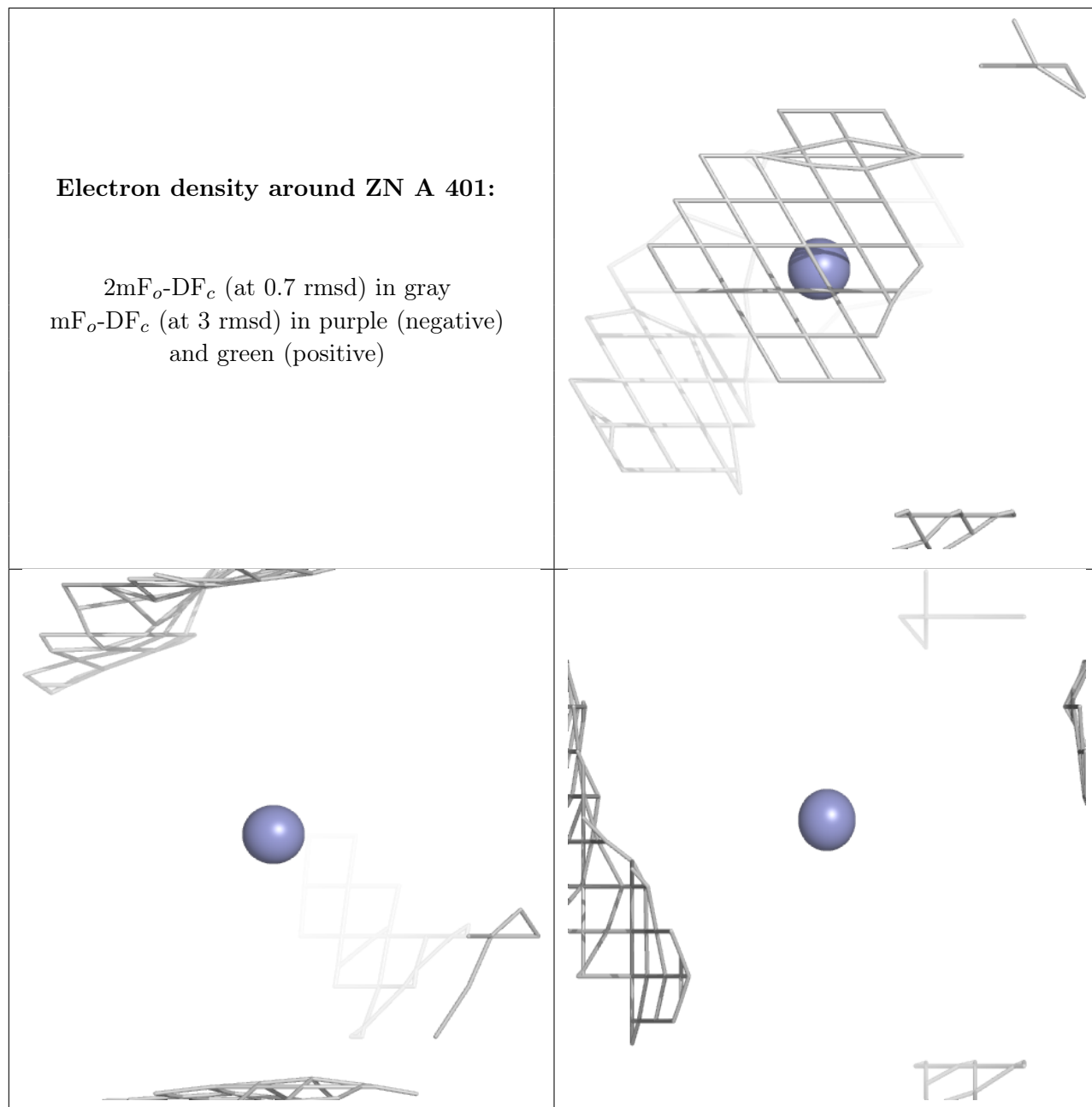
Electron density around ZN B 604:

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



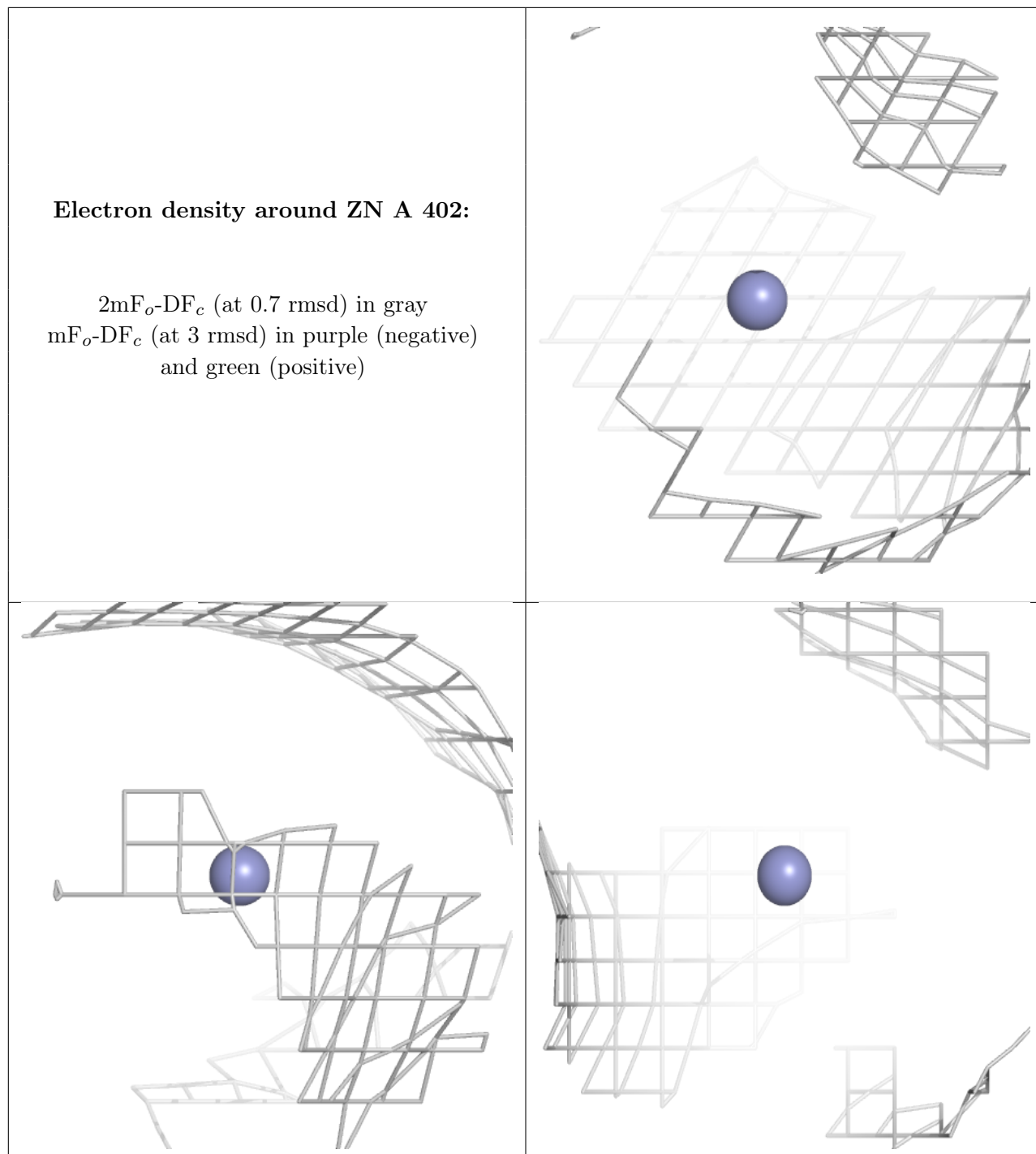
Electron density around ZN A 401:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.