



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:38 PM UTC

PDB ID : 8P90 / pdb_00008p90
Title : TARGET COMPLEX 2
Authors : Garau, G.
Deposited on : 2023-06-05
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

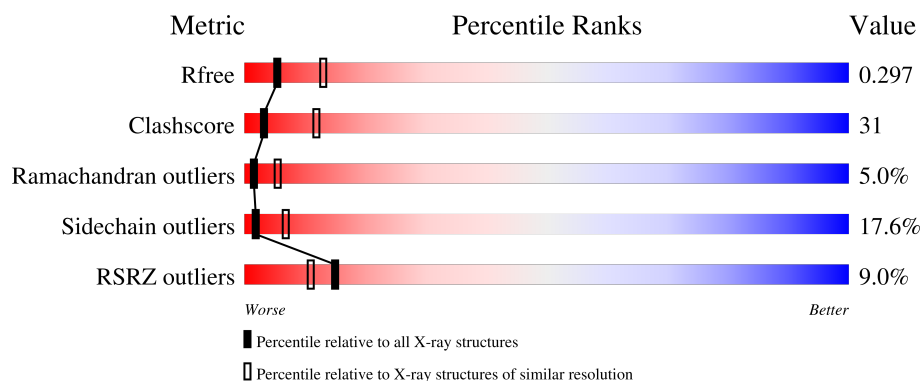
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	393	10% 29% 38% 16% • 16%
1	B	393	5% 41% 40% • • 15%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5919 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.

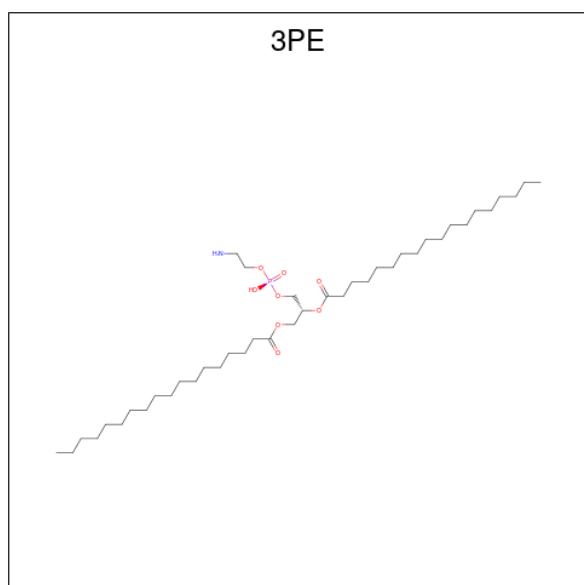
- Molecule 1 is a protein called N-acyl-phosphatidylethanolamine-hydrolyzing phospholipase D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	2	0
			2741	1775	466	486	14			
1	B	334	Total	C	N	O	S	0	3	0
			2760	1785	467	494	14			

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

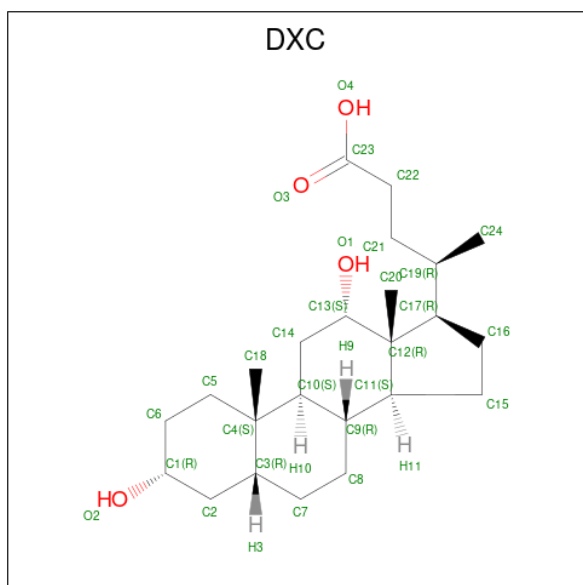
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- 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).



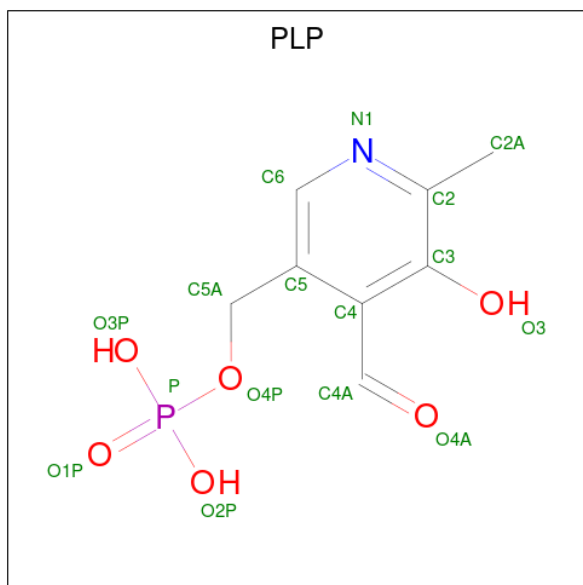
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		

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

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

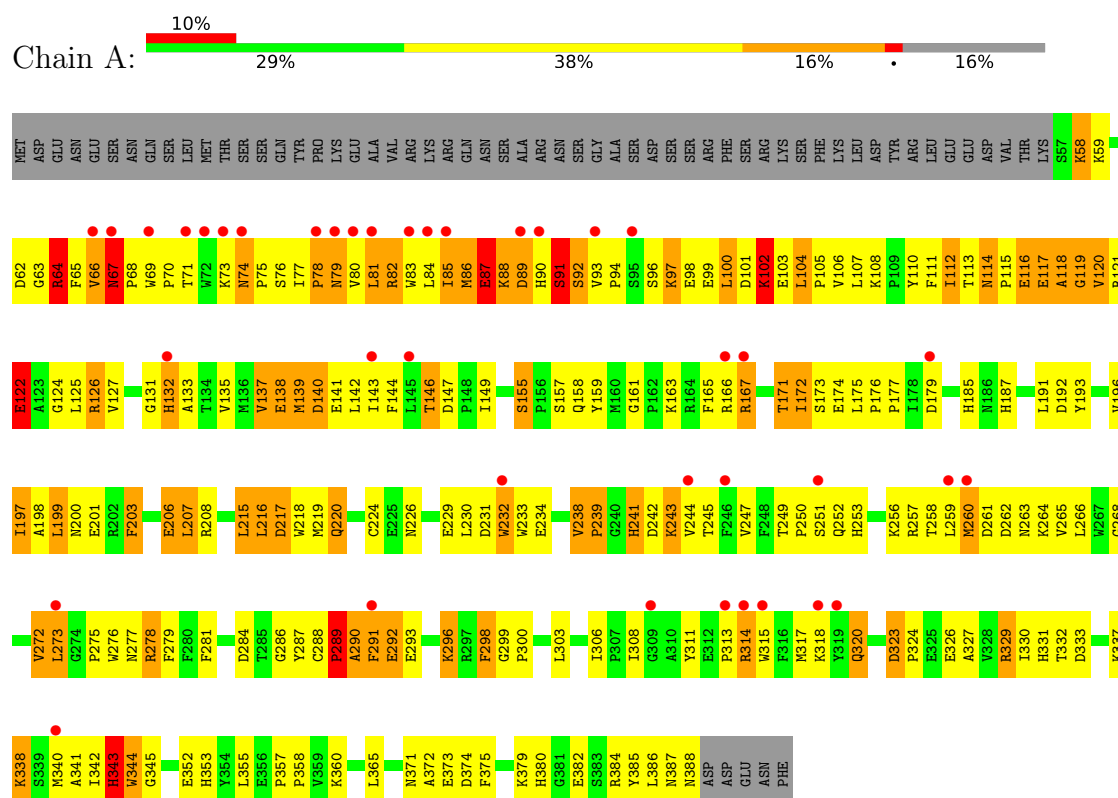
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	17	Total	O	0	0
			17	17		

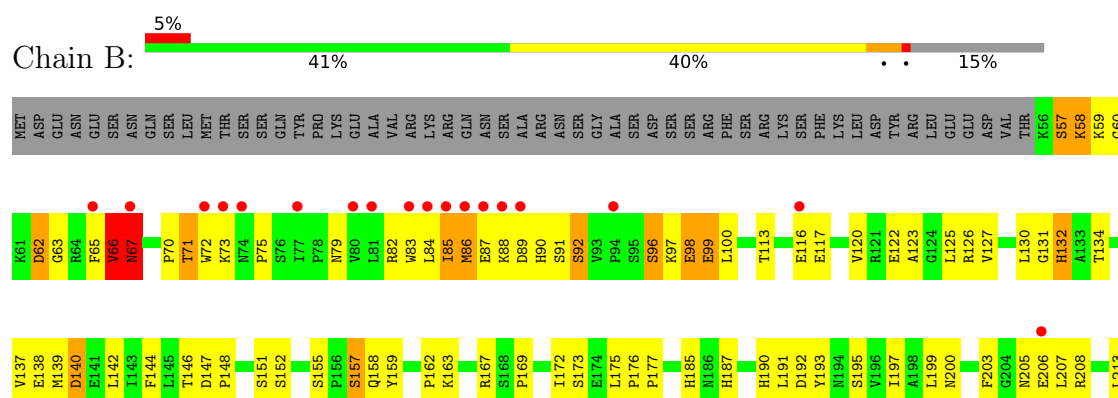
3 Residue-property plots [i](#)

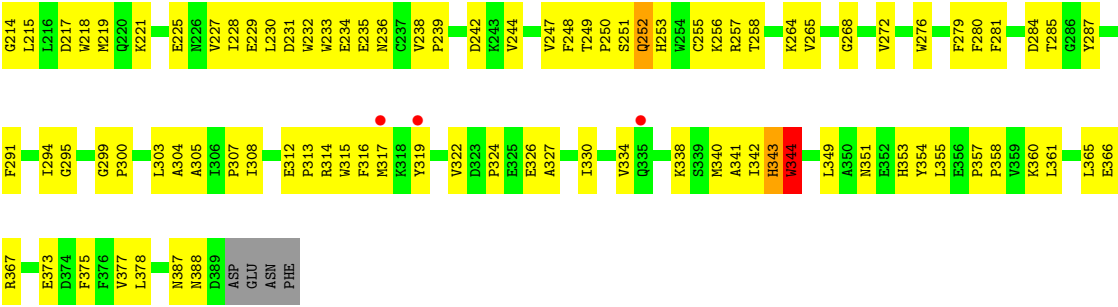
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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





R367
E373
D374
F375
F376
V377
L378
N387
N388
D389
ASP
GLU
ASN
PHE

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	94.66Å 94.66Å 441.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.28 – 2.80 46.28 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.28-2.80) 99.4 (46.28-2.80)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.271 , 0.295 0.271 , 0.297	Depositor DCC
R_{free} test set	1622 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	100.0	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 105.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5919	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: 3PE, ZN, DXC, PLP

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	0.85	2/2842 (0.1%)	1.08	6/3869 (0.2%)
1	B	0.49	0/2861	0.77	1/3896 (0.0%)
All	All	0.69	2/5703 (0.0%)	0.94	7/7765 (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	6.59	1.32	1.24
1	A	315[B]	TRP	C-O	6.59	1.32	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315[A]	TRP	CA-C-O	7.76	128.77	119.61
1	A	315[B]	TRP	CA-C-O	7.76	128.77	119.61
1	B	206	GLU	N-CA-C	-5.75	105.37	112.90
1	A	64	ARG	N-CA-C	5.55	117.70	110.43
1	A	91	SER	N-CA-C	-5.52	105.53	114.09
1	A	165	PHE	N-CA-C	-5.08	106.76	113.17
1	A	77	ILE	CA-C-O	-5.05	117.31	119.94

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	2741	0	2641	193	0
1	B	2760	0	2645	163	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	62	6	0
3	B	44	0	62	3	0
4	A	140	0	195	13	0
4	B	140	0	195	9	0
5	A	16	0	7	2	0
6	A	13	0	0	1	0
6	B	17	0	0	2	0
All	All	5919	0	5807	361	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 31.

All (361) 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:130:LEU:O	1:B:134:THR:HB	1.56	1.06
1:A:121:ARG:HD3	1:A:141:GLU:HA	1.39	1.04
1:A:92:SER:HA	1:A:353:HIS:HA	1.44	0.99
1:B:313:PRO:HD2	1:B:317:MET:HG3	1.46	0.97
1:A:59:LYS:HG3	1:A:293:GLU:HB3	1.49	0.94
1:A:203:PHE:HB2	1:A:207:LEU:HD12	1.53	0.91
4:A:405:DXC:H211	4:B:602:DXC:H81	1.56	0.88
1:A:65:PHE:HD2	1:A:68:PRO:HD2	1.39	0.86
1:A:62:ASP:HB3	1:A:232:TRP:HE1	1.39	0.84
1:B:127:VAL:HG21	1:B:340:MET:HE1	1.60	0.80
1:B:193:TYR:CZ	1:B:197:ILE:HD11	2.17	0.79
1:A:121:ARG:HH21	1:A:143:ILE:HD11	1.47	0.79
1:B:120:VAL:HG23	1:B:122:GLU:H	1.48	0.78
1:A:314:ARG:HG3	1:A:318:LYS:HE2	1.66	0.78
1:B:90:HIS:O	1:B:90:HIS:ND1	2.17	0.77
1:B:167:ARG:H	1:B:167:ARG:HD2	1.49	0.77
1:B:251:SER:HB3	1:B:268:GLY:HA2	1.68	0.76
1:A:261:ASP:HA	1:A:264:LYS:HE2	1.68	0.75
1:A:258:THR:HG21	4:A:406:DXC:H51	1.67	0.75
1:B:185:HIS:CD2	1:B:187:HIS:ND1	2.55	0.74
1:A:83:TRP:CD1	1:A:88:LYS:HB2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:LEU:HD22	1:B:234:GLU:HG2	1.71	0.72
1:A:125:LEU:HD11	1:A:137:VAL:HG12	1.71	0.72
1:B:264:LYS:NZ	6:B:701:HOH:O	2.21	0.72
1:B:214:GLY:N	1:B:229:GLU:OE2	2.21	0.71
1:A:62:ASP:HB3	1:A:232:TRP:NE1	2.06	0.70
1:A:353:HIS:HD2	1:A:355:LEU:H	1.40	0.70
1:A:353:HIS:CD2	1:A:355:LEU:H	2.09	0.69
1:B:130:LEU:HA	1:B:169:PRO:HG2	1.72	0.69
1:B:125:LEU:HD21	1:B:139:MET:HE2	1.75	0.68
1:B:152:SER:OG	1:B:163:LYS:HE2	1.94	0.68
1:B:72[A]:TRP:HE3	1:B:73:LYS:HE2	1.59	0.68
1:B:291:PHE:CD2	1:B:330:ILE:HD11	2.28	0.67
4:A:405:DXC:H211	4:B:602:DXC:H151	1.77	0.67
1:A:75:PRO:HB2	1:A:252:GLN:HE22	1.60	0.66
1:A:187:HIS:CG	3:A:403:3PE:H12	2.31	0.66
1:A:83:TRP:CE3	1:A:83:TRP:O	2.49	0.65
1:A:273:LEU:HD12	1:A:278:ARG:HG2	1.79	0.65
1:A:159:TYR:HA	1:B:193:TYR:CE2	2.31	0.65
1:A:172:ILE:O	1:A:175:LEU:HB2	1.97	0.65
1:A:258:THR:HA	3:A:403:3PE:H282	1.79	0.65
1:A:71:THR:HG22	1:A:73:LYS:HG2	1.78	0.65
1:A:185:HIS:CE1	1:A:284:ASP:HB2	2.32	0.64
1:B:218:TRP:HE3	1:B:219:MET:HE2	1.62	0.64
1:A:65:PHE:H	1:A:70:PRO:HD3	1.63	0.64
1:B:314:ARG:NH1	1:B:326:GLU:OE2	2.30	0.64
1:A:120:VAL:HG11	1:A:126:ARG:HB2	1.79	0.64
1:B:238:VAL:HG13	1:B:239:PRO:HD2	1.79	0.63
1:A:167[B]:ARG:NH1	1:B:173:SER:OG	2.30	0.63
1:A:126:ARG:HB3	1:A:138:GLU:HG3	1.80	0.63
1:B:65:PHE:H	1:B:70:PRO:HD3	1.64	0.63
1:B:305:ALA:HB1	1:B:342:ILE:HD13	1.81	0.63
1:A:74:ASN:C	1:A:76:SER:H	2.07	0.63
1:A:90:HIS:CD2	1:A:93:VAL:H	2.18	0.62
1:A:127:VAL:HG11	1:A:303:LEU:HD23	1.81	0.61
1:B:258:THR:HB	4:B:602:DXC:H1	1.81	0.61
1:A:105:PRO:HG2	1:A:379:LYS:HD3	1.82	0.61
1:A:241:HIS:HA	1:A:243:LYS:HE2	1.83	0.61
1:B:365:LEU:HD11	1:B:375:PHE:HB3	1.80	0.61
1:A:115:PRO:O	1:A:116:GLU:C	2.43	0.61
1:A:173:SER:HB3	1:B:167:ARG:HH22	1.65	0.61
1:B:330:ILE:O	1:B:334:VAL:HG12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:HD2	4:A:408:DXC:H3	1.84	0.60
1:A:323:ASP:H	1:A:326:GLU:HB2	1.65	0.60
1:A:272:VAL:HG13	1:A:279:PHE:HB3	1.84	0.60
1:A:64:ARG:HG2	1:A:69:TRP:CZ3	2.37	0.60
1:A:387:ASN:O	1:A:388:ASN:HB2	2.01	0.60
1:A:308:ILE:O	1:A:357:PRO:HB3	2.02	0.60
1:A:232:TRP:CE3	1:A:250:PRO:HA	2.36	0.59
1:A:251:SER:HB2	1:A:268:GLY:HA2	1.84	0.59
1:B:218:TRP:CE3	1:B:219:MET:HE2	2.37	0.59
1:B:324:PRO:HG2	1:B:360:LYS:HB2	1.85	0.59
1:A:62:ASP:OD1	1:A:63:GLY:C	2.46	0.59
1:A:296:LYS:HZ2	1:A:296:LYS:HA	1.67	0.59
1:A:96:SER:HB2	1:A:99:GLU:HB2	1.85	0.58
1:B:313:PRO:O	1:B:316:PHE:N	2.36	0.58
1:B:83:TRP:HA	1:B:88:LYS:HZ3	1.67	0.58
1:A:355:LEU:O	1:A:358:PRO:HD2	2.03	0.58
1:A:139:MET:O	1:A:140:ASP:C	2.47	0.58
1:A:230:LEU:HD23	1:A:234:GLU:HB3	1.86	0.58
1:B:59:LYS:O	1:B:59:LYS:HG3	2.03	0.57
1:B:280:PHE:CE1	1:B:294:ILE:HG21	2.38	0.57
1:B:308:ILE:HG12	1:B:341:ALA:HB1	1.84	0.57
1:B:312:GLU:HB3	1:B:313:PRO:HD3	1.85	0.57
1:A:110:TYR:C	1:A:112:ILE:H	2.13	0.57
1:A:64:ARG:HA	1:A:70:PRO:CD	2.34	0.57
1:B:256:LYS:HG2	3:B:605:3PE:H221	1.86	0.57
1:A:110:TYR:HE2	1:A:118:ALA:H	1.52	0.57
1:A:159:TYR:HA	1:B:193:TYR:HE2	1.67	0.57
1:A:290:ALA:O	1:A:291:PHE:C	2.47	0.57
1:B:213:LEU:HD23	1:B:229:GLU:HG2	1.87	0.57
1:A:121:ARG:NH2	1:A:143:ILE:HD11	2.18	0.57
1:B:75:PRO:O	1:B:319:TYR:HD2	1.87	0.57
1:B:147:ASP:OD2	1:B:190:HIS:HB3	2.04	0.57
1:A:58:LYS:HG3	1:A:59:LYS:HD3	1.87	0.56
1:A:74:ASN:O	1:A:76:SER:N	2.39	0.56
1:B:83:TRP:HE1	1:B:349:LEU:HA	1.70	0.56
1:B:85:ILE:O	1:B:86:MET:C	2.48	0.56
1:B:191:LEU:O	1:B:257:ARG:NH2	2.39	0.56
1:A:289:PRO:O	1:A:290:ALA:C	2.47	0.56
1:B:123:ALA:HA	1:B:276:TRP:CD1	2.41	0.56
1:A:215:LEU:O	1:A:216:LEU:C	2.48	0.56
1:A:353:HIS:CD2	1:A:355:LEU:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:HG12	1:A:137:VAL:HG13	1.87	0.55
1:A:244:VAL:HG12	1:A:275:PRO:HD2	1.88	0.55
1:B:312:GLU:HG2	1:B:351:ASN:HB2	1.87	0.55
1:A:116:GLU:O	1:A:117:GLU:C	2.49	0.55
1:A:65:PHE:N	1:A:70:PRO:HD3	2.20	0.55
1:A:74:ASN:C	1:A:76:SER:N	2.60	0.55
1:B:213:LEU:HA	1:B:229:GLU:HG2	1.89	0.55
1:B:65:PHE:O	1:B:66:VAL:C	2.49	0.55
1:A:215:LEU:HD13	1:A:219:MET:HE3	1.89	0.55
1:B:120:VAL:HG11	1:B:138:GLU:C	2.32	0.54
1:A:232:TRP:O	1:A:233:TRP:HB2	2.06	0.54
1:B:322:VAL:HB	1:B:326:GLU:HB2	1.90	0.54
1:A:139:MET:HG2	1:A:144:PHE:HE1	1.73	0.54
1:A:143:ILE:H	1:A:179:ASP:CG	2.16	0.54
1:B:249:THR:HB	1:B:294:ILE:HG12	1.89	0.53
1:B:82:ARG:HG3	4:B:608:DXC:H1	1.90	0.53
1:A:114:ASN:O	1:A:117:GLU:HG3	2.07	0.53
1:B:235:GLU:HB3	1:B:247:VAL:HG22	1.91	0.53
1:A:65:PHE:O	1:A:66:VAL:C	2.50	0.53
1:A:133:ALA:HB1	1:A:281:PHE:HZ	1.73	0.53
1:A:371:ASN:OD1	1:A:372:ALA:N	2.41	0.53
1:B:130:LEU:O	1:B:134:THR:CB	2.44	0.53
1:B:192:ASP:HB3	1:B:195:SER:HB2	1.90	0.53
1:B:291:PHE:CD2	1:B:330:ILE:CD1	2.91	0.53
1:A:142:LEU:HD21	1:A:241:HIS:HB2	1.91	0.53
1:A:185:HIS:CD2	1:A:187:HIS:ND1	2.77	0.52
1:B:97:LYS:HA	1:B:100:LEU:HD13	1.92	0.52
1:B:205:ASN:OD1	1:B:225:GLU:HB2	2.09	0.52
1:B:343:HIS:O	1:B:344:TRP:CD1	2.63	0.52
1:A:65:PHE:CD2	1:A:68:PRO:HD2	2.31	0.52
1:A:146:THR:O	1:A:147:ASP:C	2.53	0.52
1:B:84:LEU:HD21	4:B:608:DXC:H52	1.91	0.51
1:A:338:LYS:HA	1:A:374:ASP:O	2.11	0.51
1:A:256:LYS:HD3	3:A:403:3PE:H242	1.93	0.51
1:B:151:SER:OG	1:B:192:ASP:OD2	2.21	0.51
1:A:326:GLU:O	1:A:330:ILE:HG12	2.10	0.51
1:B:232:TRP:CZ3	1:B:250:PRO:HA	2.45	0.51
1:A:74:ASN:ND2	1:A:75:PRO:HD3	2.26	0.51
1:B:142:LEU:CD1	1:B:244:VAL:HG11	2.41	0.51
1:B:227:VAL:O	1:B:228:ILE:HD12	2.11	0.51
1:B:255:CYS:SG	1:B:265:VAL:HG23	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:LYS:HZ2	1:B:373:GLU:C	2.19	0.50
1:B:91:SER:HB2	1:B:351:ASN:O	2.10	0.50
1:B:305:ALA:HB1	1:B:342:ILE:HG21	1.93	0.50
1:B:92:SER:HB3	1:B:354:TYR:H	1.75	0.50
5:A:409:PLP:H5A1	1:B:151:SER:HA	1.92	0.50
1:B:134:THR:HG23	1:B:148:PRO:HA	1.94	0.50
1:B:228:ILE:HG21	1:B:236:ASN:HD22	1.77	0.50
1:A:218:TRP:NE1	4:A:404:DXC:H3	2.27	0.50
1:A:287:TYR:HE2	1:A:329:ARG:HB2	1.75	0.50
1:B:142:LEU:HD11	1:B:244:VAL:HG11	1.94	0.50
1:A:102:LYS:N	1:A:102:LYS:HD2	2.26	0.50
1:A:71:THR:HG21	1:A:252:GLN:HG3	1.93	0.50
1:B:65:PHE:N	1:B:70:PRO:HD3	2.27	0.50
1:B:92:SER:HB3	1:B:354:TYR:N	2.27	0.50
1:A:314:ARG:HE	1:A:318:LYS:NZ	2.10	0.50
1:B:299:GLY:HA2	1:B:300:PRO:C	2.37	0.50
1:A:217:ASP:O	1:A:218:TRP:C	2.54	0.49
1:A:365:LEU:HD11	1:A:375:PHE:HB3	1.93	0.49
1:B:134:THR:HA	1:B:146:THR:O	2.12	0.49
4:A:406:DXC:H182	4:B:607:DXC:H222	1.93	0.49
1:A:218:TRP:HE3	1:A:219:MET:HE2	1.77	0.49
1:A:317:MET:HE1	3:A:403:3PE:H122	1.94	0.49
1:A:82:ARG:HB2	4:A:408:DXC:H51	1.94	0.49
1:B:187:HIS:CG	3:B:605:3PE:H12	2.48	0.49
4:A:406:DXC:H71	4:B:607:DXC:C23	2.43	0.49
1:B:193:TYR:CE2	1:B:197:ILE:HD11	2.47	0.49
1:B:125:LEU:CD2	1:B:139:MET:HB3	2.42	0.48
1:B:307:PRO:HA	1:B:342:ILE:O	2.12	0.48
1:A:118:ALA:O	1:A:120:VAL:N	2.46	0.48
1:A:340:MET:O	1:A:341:ALA:HB3	2.14	0.48
1:A:142:LEU:HD21	1:A:241:HIS:CB	2.43	0.48
1:A:124:GLY:HA3	1:A:387:ASN:HA	1.95	0.48
1:A:384:ARG:HG2	1:A:386:LEU:HD11	1.94	0.48
1:B:233:TRP:N	1:B:248:PHE:O	2.46	0.48
1:A:290:ALA:O	1:A:293:GLU:N	2.47	0.48
1:A:65:PHE:CG	1:A:66:VAL:N	2.82	0.48
1:B:272:VAL:HG22	1:B:279:PHE:HB3	1.95	0.48
1:A:64:ARG:HA	1:A:70:PRO:HD2	1.96	0.48
1:A:137:VAL:HB	1:A:144:PHE:CZ	2.49	0.48
1:A:231:ASP:H	1:A:234:GLU:CD	2.22	0.48
1:B:341:ALA:CB	1:B:377:VAL:HG12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ASP:O	1:A:324:PRO:C	2.56	0.47
1:B:185:HIS:CE1	1:B:284:ASP:HB2	2.49	0.47
1:B:65:PHE:CD2	1:B:66:VAL:HG22	2.49	0.47
1:A:59:LYS:HE3	1:A:293:GLU:HA	1.96	0.47
1:A:231:ASP:O	1:A:232:TRP:C	2.57	0.47
6:A:507:HOH:O	1:B:172:ILE:HG12	2.14	0.47
1:B:85:ILE:HB	1:B:89:ASP:HB3	1.96	0.47
1:A:296:LYS:HA	1:A:296:LYS:NZ	2.30	0.47
1:B:191:LEU:HD11	1:B:219:MET:HE1	1.96	0.47
1:A:140:ASP:O	1:A:141:GLU:HB2	2.14	0.47
4:A:405:DXC:C21	4:B:602:DXC:H151	2.44	0.47
1:B:84:LEU:O	1:B:88:LYS:HD2	2.15	0.47
1:B:96:SER:HB3	1:B:98:GLU:HG2	1.96	0.47
1:A:288:CYS:O	1:A:289:PRO:C	2.58	0.47
1:A:289:PRO:O	1:A:291:PHE:N	2.47	0.47
1:A:317:MET:O	1:A:318:LYS:C	2.57	0.47
1:A:241:HIS:CD2	1:A:241:HIS:H	2.33	0.47
1:B:63:GLY:O	1:B:70:PRO:HD2	2.14	0.47
1:A:185:HIS:CD2	1:A:187:HIS:CG	3.02	0.47
1:A:185:HIS:HD2	1:A:187:HIS:CG	2.33	0.47
1:A:299:GLY:HA2	1:A:300:PRO:C	2.39	0.47
1:A:371:ASN:ND2	1:A:373:GLU:HG3	2.29	0.47
1:B:116[B]:GLU:OE1	1:B:117:GLU:N	2.44	0.47
1:B:131:GLY:O	1:B:132:HIS:C	2.58	0.46
1:A:81:LEU:HD11	4:A:408:DXC:H62	1.97	0.46
4:A:408:DXC:H243	4:A:408:DXC:H221	1.71	0.46
1:B:327:ALA:O	1:B:330:ILE:HB	2.15	0.46
1:B:200:ASN:O	1:B:203:PHE:O	2.34	0.46
1:A:91:SER:O	1:A:93:VAL:HG23	2.15	0.46
1:A:311:TYR:HE2	1:A:357:PRO:HG3	1.80	0.46
1:B:316:PHE:CD1	1:B:316:PHE:C	2.93	0.46
1:A:64:ARG:HA	1:A:70:PRO:HD3	1.97	0.46
1:A:88:LYS:O	1:A:88:LYS:HG2	2.16	0.46
1:A:110:TYR:C	1:A:112:ILE:N	2.74	0.46
1:A:100:LEU:HD12	1:A:166:ARG:NE	2.31	0.46
1:A:119:GLY:HA2	1:A:121:ARG:CZ	2.46	0.46
1:A:200:ASN:O	1:A:201:GLU:C	2.58	0.46
1:B:185:HIS:CD2	1:B:253:HIS:CD2	3.04	0.46
1:B:83:TRP:CZ2	1:B:162:PRO:HB3	2.50	0.45
1:B:84:LEU:O	1:B:85:ILE:C	2.59	0.45
1:A:196:VAL:O	1:A:197:ILE:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ARG:HD2	1:A:314:ARG:HA	1.51	0.45
1:A:326:GLU:HA	1:A:329:ARG:HG3	1.98	0.45
1:B:280:PHE:O	1:B:304:ALA:HA	2.16	0.45
1:B:281:PHE:HD1	1:B:305:ALA:HB3	1.81	0.45
1:A:171:THR:HG23	1:A:174:GLU:CD	2.41	0.45
1:A:289:PRO:O	1:A:292:GLU:HG2	2.17	0.45
1:B:175:LEU:HB2	1:B:176:PRO:HD2	1.98	0.45
1:A:157:SER:OG	1:A:158:GLN:N	2.50	0.45
1:A:198:ALA:O	1:A:199:LEU:C	2.60	0.45
1:A:330:ILE:O	1:A:331:HIS:C	2.59	0.45
1:A:131:GLY:O	1:A:132:HIS:C	2.60	0.45
1:A:216:LEU:O	1:A:217:ASP:C	2.59	0.45
1:B:99:GLU:HG3	1:B:100:LEU:N	2.32	0.45
1:A:88:LYS:HD3	1:A:88:LYS:C	2.40	0.45
1:B:96:SER:O	1:B:97:LYS:C	2.60	0.45
1:A:67:ASN:HB2	1:A:68:PRO:HD3	1.99	0.45
1:A:86:MET:HE2	1:A:87:GLU:HG2	1.99	0.45
1:B:62:ASP:OD1	1:B:62:ASP:N	2.49	0.44
1:B:65:PHE:CG	1:B:66:VAL:N	2.85	0.44
1:B:98:GLU:H	1:B:98:GLU:CD	2.25	0.44
1:B:185:HIS:HD2	1:B:187:HIS:ND1	2.02	0.44
1:A:62:ASP:HA	1:A:63:GLY:HA3	1.79	0.44
1:A:258:THR:OG1	1:A:259:LEU:N	2.50	0.44
1:B:207:LEU:HD12	1:B:207:LEU:HA	1.63	0.44
1:A:139:MET:HE2	1:A:139:MET:HB2	1.72	0.44
1:A:233:TRP:CE3	1:A:233:TRP:HA	2.53	0.44
1:A:247:VAL:HG11	1:A:298:PHE:CZ	2.53	0.44
1:A:329:ARG:HE	1:A:329:ARG:HB3	1.53	0.44
1:B:84:LEU:O	1:B:86:MET:N	2.50	0.44
1:B:256:LYS:HE3	1:B:258:THR:O	2.18	0.44
1:B:313:PRO:HB2	1:B:316:PHE:HB3	2.00	0.44
1:A:107:LEU:HD12	1:A:382:GLU:HB2	1.99	0.44
1:B:84:LEU:C	1:B:86:MET:N	2.72	0.44
1:B:217:ASP:O	1:B:221:LYS:HG2	2.18	0.44
1:B:185:HIS:CE1	1:B:190:HIS:CD2	3.06	0.44
1:B:308:ILE:HD12	1:B:357:PRO:CB	2.47	0.44
1:A:262:ASP:O	1:A:263:ASN:C	2.61	0.44
5:A:409:PLP:H5A2	5:A:409:PLP:H4A	1.71	0.44
1:B:208:ARG:NH2	1:B:228:ILE:HD11	2.33	0.44
1:A:324:PRO:HG2	1:A:360:LYS:HB3	2.00	0.44
1:A:117:GLU:O	1:A:118:ALA:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLU:HG3	1:A:385:TYR:OH	2.18	0.44
1:B:97:LYS:O	1:B:100:LEU:N	2.50	0.44
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.76	0.44
1:B:229:GLU:O	1:B:230:LEU:HD23	2.18	0.44
1:A:172:ILE:HA	1:A:175:LEU:HD12	1.99	0.43
1:A:253:HIS:CE1	1:A:284:ASP:HB3	2.53	0.43
1:A:318:LYS:HA	1:A:318:LYS:HD3	1.83	0.43
1:B:291:PHE:CE2	1:B:330:ILE:HD11	2.52	0.43
1:A:260:MET:C	1:A:262:ASP:H	2.26	0.43
1:B:185:HIS:CD2	1:B:253:HIS:HD2	2.36	0.43
1:A:111:PHE:CD2	1:A:176:PRO:HD3	2.54	0.43
1:B:97:LYS:O	1:B:98:GLU:C	2.60	0.43
1:A:345:GLY:O	1:A:380:HIS:HE1	2.00	0.43
3:A:403:3PE:H3A2	4:B:601:DXC:H21	2.00	0.43
1:B:139:MET:HE1	1:B:279:PHE:CB	2.48	0.43
1:B:215:LEU:HD12	1:B:215:LEU:HA	1.84	0.43
1:A:112:ILE:O	1:A:115:PRO:HD3	2.19	0.43
1:A:193:TYR:CE2	1:B:159:TYR:HA	2.54	0.43
1:A:324:PRO:O	1:A:327:ALA:HB3	2.19	0.43
1:B:285:THR:HG21	1:B:291:PHE:CZ	2.54	0.43
1:B:340:MET:HE3	1:B:340:MET:HB3	1.73	0.43
1:B:287:TYR:HB2	1:B:326:GLU:OE1	2.18	0.43
1:A:192:ASP:O	1:A:196:VAL:HG23	2.19	0.43
1:B:139:MET:HE1	1:B:279:PHE:HB3	2.01	0.43
1:A:100:LEU:O	1:A:104:LEU:N	2.52	0.42
1:A:199:LEU:HD13	1:A:199:LEU:HA	1.82	0.42
1:A:219:MET:O	1:A:220:GLN:C	2.62	0.42
1:B:177:PRO:HA	1:B:203:PHE:HE2	1.82	0.42
1:A:120:VAL:C	1:A:122:GLU:H	2.27	0.42
1:A:216:LEU:HB2	1:A:229:GLU:CD	2.44	0.42
1:A:241:HIS:CD2	1:A:241:HIS:N	2.87	0.42
1:A:313:PRO:O	1:A:317:MET:HG2	2.19	0.42
1:B:75:PRO:HD2	1:B:252:GLN:NE2	2.34	0.42
1:B:127:VAL:HG21	1:B:340:MET:CE	2.39	0.42
1:B:227:VAL:C	1:B:228:ILE:HD12	2.44	0.42
1:A:81:LEU:HD13	1:A:82:ARG:H	1.84	0.42
4:A:404:DXC:H181	4:A:407:DXC:C23	2.49	0.42
1:B:63:GLY:C	1:B:70:PRO:HD2	2.44	0.42
1:A:187:HIS:ND1	3:A:403:3PE:H12	2.34	0.42
1:A:191:LEU:HD23	1:A:257:ARG:HD2	1.99	0.42
1:A:71:THR:C	1:A:73:LYS:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:THR:HG21	1:B:252:GLN:HG2	2.01	0.42
1:A:110:TYR:OH	1:A:118:ALA:HA	2.19	0.42
1:A:343:HIS:O	1:A:344:TRP:CD1	2.72	0.42
1:B:127:VAL:HG11	1:B:303:LEU:HD11	2.02	0.42
1:B:232:TRP:CE3	1:B:250:PRO:HA	2.55	0.42
1:A:206:GLU:H	1:A:206:GLU:CD	2.26	0.42
1:A:238:VAL:O	1:A:239:PRO:C	2.62	0.42
1:A:292:GLU:O	1:A:293:GLU:C	2.63	0.42
1:B:92:SER:HB3	1:B:353:HIS:HA	2.01	0.42
1:B:367:ARG:HE	1:B:367:ARG:HB3	1.49	0.42
1:A:110:TYR:CE2	1:A:117:GLU:HB2	2.55	0.42
1:A:155:SER:CB	1:A:161:GLY:HA3	2.50	0.42
1:A:253:HIS:HB2	1:A:284:ASP:O	2.20	0.41
1:B:57:SER:O	1:B:58:LYS:C	2.63	0.41
1:A:287:TYR:CE2	1:A:329:ARG:HB2	2.54	0.41
4:A:408:DXC:H201	4:A:408:DXC:H142	1.84	0.41
1:B:316:PHE:C	1:B:316:PHE:HD1	2.29	0.41
1:B:213:LEU:HD12	1:B:231:ASP:CG	2.45	0.41
1:B:315:TRP:NE1	6:B:705:HOH:O	2.45	0.41
1:A:259:LEU:O	1:A:260:MET:HB2	2.21	0.41
1:A:311:TYR:CE2	1:A:357:PRO:HG3	2.55	0.41
1:B:140:ASP:OD1	1:B:140:ASP:N	2.53	0.41
1:B:65:PHE:HB2	1:B:70:PRO:HG3	2.02	0.41
1:B:162:PRO:HG3	3:B:605:3PE:H331	2.02	0.41
1:A:207:LEU:O	1:A:226:ASN:HB3	2.21	0.41
1:A:252:GLN:HB3	1:A:286:GLY:H	1.86	0.41
1:B:66:VAL:HG23	1:B:67:ASN:H	1.86	0.41
1:B:357:PRO:HB2	1:B:358:PRO:HD3	2.01	0.41
1:B:387:ASN:OD1	1:B:388:ASN:N	2.54	0.41
1:A:353:HIS:HD2	1:A:355:LEU:N	2.14	0.41
1:B:234:GLU:O	1:B:247:VAL:HA	2.20	0.41
1:A:273:LEU:HA	1:A:278:ARG:HG2	2.01	0.41
1:B:147:ASP:OD2	1:B:190:HIS:ND1	2.53	0.41
1:A:104:LEU:HD22	1:A:104:LEU:HA	1.78	0.41
1:A:114:ASN:O	1:A:115:PRO:C	2.63	0.41
1:A:200:ASN:ND2	1:A:224:CYS:HA	2.36	0.41
1:B:295:GLY:HA3	1:B:334:VAL:HA	2.03	0.41
1:B:330:ILE:HG23	1:B:330:ILE:HD12	1.60	0.41
1:A:317:MET:HA	1:A:320:GLN:OE1	2.21	0.41
1:B:117:GLU:O	1:B:126:ARG:NH2	2.54	0.40
1:B:137:VAL:HB	1:B:144:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:SER:HB3	1:A:98:GLU:OE2	2.21	0.40
1:B:272:VAL:CG2	1:B:279:PHE:HB3	2.51	0.40
1:B:313:PRO:O	1:B:314:ARG:C	2.65	0.40
1:A:69:TRP:CD2	1:A:266:LEU:HD13	2.56	0.40
1:A:116:GLU:HG2	1:A:117:GLU:H	1.86	0.40
1:A:179:ASP:OD1	1:A:179:ASP:N	2.54	0.40
1:B:157:SER:OG	1:B:158:GLN:N	2.55	0.40
1:B:303:LEU:HD23	1:B:303:LEU:HA	1.83	0.40
1:A:103:GLU:O	1:A:105:PRO:HD3	2.21	0.40
1:A:110:TYR:CG	1:A:111:PHE:N	2.90	0.40
1:B:125:LEU:CD2	1:B:139:MET:HE2	2.47	0.40
1:B:308:ILE:O	1:B:357:PRO:HB3	2.21	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	332/393 (84%)	237 (71%)	70 (21%)	25 (8%)	1	2
1	B	335/393 (85%)	315 (94%)	12 (4%)	8 (2%)	4	17
All	All	667/786 (85%)	552 (83%)	82 (12%)	33 (5%)	1	6

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	A	85	ILE
1	A	89	ASP
1	A	116	GLU
1	A	117	GLU
1	A	122	GLU

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Mol	Chain	Res	Type
1	A	290	ALA
1	B	66	VAL
1	A	66	VAL
1	A	119	GLY
1	B	60	GLY
1	B	86	MET
1	A	67	ASN
1	A	79	ASN
1	A	87	GLU
1	A	118	ALA
1	A	239	PRO
1	B	58	LYS
1	B	344	TRP
1	A	140	ASP
1	A	289	PRO
1	B	67	ASN
1	A	203	PHE
1	A	291	PHE
1	A	343	HIS
1	A	97	LYS
1	A	102	LYS
1	A	177	PRO
1	A	197	ILE
1	A	216	LEU
1	B	132	HIS
1	A	94	PRO
1	B	85	ILE

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	297/352 (84%)	216 (73%)	81 (27%)	0	1
1	B	299/352 (85%)	275 (92%)	24 (8%)	11	34
All	All	596/704 (85%)	491 (82%)	105 (18%)	2	7

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	64	ARG
1	A	67	ASN
1	A	74	ASN
1	A	78	PRO
1	A	79	ASN
1	A	80	VAL
1	A	81	LEU
1	A	82	ARG
1	A	84	LEU
1	A	85	ILE
1	A	86	MET
1	A	87	GLU
1	A	88	LYS
1	A	89	ASP
1	A	91	SER
1	A	92	SER
1	A	97	LYS
1	A	100	LEU
1	A	101	ASP
1	A	102	LYS
1	A	104	LEU
1	A	106	VAL
1	A	108	LYS
1	A	112	ILE
1	A	113	THR
1	A	114	ASN
1	A	120	VAL
1	A	122	GLU
1	A	126	ARG
1	A	132	HIS
1	A	135	VAL
1	A	137	VAL
1	A	138	GLU
1	A	139	MET
1	A	146	THR
1	A	149	ILE
1	A	155	SER
1	A	163	LYS
1	A	167[A]	ARG
1	A	167[B]	ARG
1	A	171	THR

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Mol	Chain	Res	Type
1	A	172	ILE
1	A	199	LEU
1	A	206	GLU
1	A	207	LEU
1	A	208	ARG
1	A	215	LEU
1	A	217	ASP
1	A	220	GLN
1	A	232	TRP
1	A	238	VAL
1	A	241	HIS
1	A	242	ASP
1	A	243	LYS
1	A	245	THR
1	A	249	THR
1	A	260	MET
1	A	265	VAL
1	A	272	VAL
1	A	273	LEU
1	A	276	TRP
1	A	277	ASN
1	A	278	ARG
1	A	289	PRO
1	A	292	GLU
1	A	296	LYS
1	A	298	PHE
1	A	306	ILE
1	A	314	ARG
1	A	320	GLN
1	A	323	ASP
1	A	329	ARG
1	A	332	THR
1	A	333	ASP
1	A	337	LYS
1	A	338	LYS
1	A	342	ILE
1	A	343	HIS
1	A	344	TRP
1	A	352	GLU
1	B	57	SER
1	B	62	ASP
1	B	66	VAL

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Mol	Chain	Res	Type
1	B	67	ASN
1	B	71	THR
1	B	79	ASN
1	B	87	GLU
1	B	92	SER
1	B	96	SER
1	B	98	GLU
1	B	99	GLU
1	B	113	THR
1	B	140	ASP
1	B	155	SER
1	B	157	SER
1	B	199	LEU
1	B	242	ASP
1	B	252	GLN
1	B	343	HIS
1	B	344	TRP
1	B	355	LEU
1	B	361	LEU
1	B	366	GLU
1	B	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	HIS
1	A	252	GLN
1	A	335	GLN
1	A	353	HIS
1	B	114	ASN
1	B	236	ASN
1	B	252	GLN
1	B	277	ASN
1	B	353	HIS
1	B	380	HIS

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	0.72	2 (4%)
4	DXC	A	407	-	31,31,31	0.62	0	49,49,49	1.29	4 (8%)
5	PLP	A	409	-	16,16,16	2.82	5 (31%)	20,23,23	3.09	7 (35%)
4	DXC	B	608	-	31,31,31	0.68	0	49,49,49	1.17	4 (8%)
4	DXC	A	408	-	31,31,31	0.62	0	49,49,49	1.57	8 (16%)
3	3PE	A	403	2	43,43,50	0.58	0	46,48,55	0.74	2 (4%)
4	DXC	A	405	-	31,31,31	0.73	1 (3%)	49,49,49	1.64	10 (20%)
4	DXC	B	601	-	31,31,31	0.64	1 (3%)	49,49,49	1.70	12 (24%)
4	DXC	B	606	-	31,31,31	0.57	0	49,49,49	1.00	1 (2%)
4	DXC	B	607	-	31,31,31	0.72	0	49,49,49	1.30	7 (14%)
4	DXC	B	602	-	31,31,31	0.70	0	49,49,49	1.54	9 (18%)
4	DXC	A	404	-	31,31,31	0.64	1 (3%)	49,49,49	0.88	2 (4%)
4	DXC	A	406	-	31,31,31	0.67	0	49,49,49	1.41	6 (12%)

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	-	22/47/47/54	-
4	DXC	A	407	-	-	0/9/71/71	0/4/4/4
5	PLP	A	409	-	-	0/8/8/8	0/1/1/1
4	DXC	B	608	-	-	2/9/71/71	0/4/4/4
4	DXC	A	408	-	-	4/9/71/71	0/4/4/4
3	3PE	A	403	2	-	18/47/47/54	-
4	DXC	A	405	-	-	3/9/71/71	0/4/4/4
4	DXC	B	601	-	-	0/9/71/71	0/4/4/4
4	DXC	B	606	-	-	7/9/71/71	0/4/4/4
4	DXC	B	607	-	-	2/9/71/71	0/4/4/4
4	DXC	B	602	-	-	2/9/71/71	0/4/4/4
4	DXC	A	404	-	-	3/9/71/71	0/4/4/4
4	DXC	A	406	-	-	7/9/71/71	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	409	PLP	C3-C2	-8.58	1.32	1.41
5	A	409	PLP	C4-C4A	5.62	1.59	1.46
5	A	409	PLP	C2-N1	2.56	1.38	1.33
4	A	405	DXC	C22-C23	2.13	1.55	1.50
4	B	601	DXC	C22-C23	2.08	1.55	1.50
5	A	409	PLP	O4A-C4A	2.04	1.28	1.21
4	A	404	DXC	C22-C23	2.03	1.55	1.50
5	A	409	PLP	C6-N1	2.01	1.38	1.34

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	409	PLP	C4-C3-C2	-6.92	116.25	120.14
5	A	409	PLP	C3-C4-C5	6.63	123.60	118.28
5	A	409	PLP	C3-C4-C4A	5.59	127.53	119.84
5	A	409	PLP	O4A-C4A-C4	-4.95	113.06	124.80
4	A	406	DXC	C5-C4-C10	-4.59	104.21	111.34
4	B	602	DXC	C12-C11-C9	-4.41	109.94	114.69
5	A	409	PLP	C2A-C2-C3	-4.25	115.82	120.80
4	A	408	DXC	C4-C10-C9	4.24	116.73	112.43
4	A	405	DXC	C20-C12-C13	4.22	113.28	109.06
4	A	405	DXC	O1-C13-C12	-4.20	103.92	111.02
4	A	405	DXC	C17-C12-C13	-4.00	114.07	117.67
4	B	601	DXC	C5-C6-C1	3.99	115.76	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	DXC	C3-C2-C1	3.93	118.63	112.71
4	A	408	DXC	C14-C13-C12	-3.89	107.31	111.26
4	A	407	DXC	O1-C13-C12	-3.55	105.03	111.02
4	B	602	DXC	C15-C11-C12	3.35	106.79	103.54
4	A	406	DXC	C11-C9-C10	-3.31	104.76	109.09
4	A	408	DXC	C16-C17-C12	-3.24	100.39	103.54
4	B	601	DXC	C2-C3-C4	3.24	116.11	112.66
4	B	602	DXC	C8-C9-C10	3.20	114.35	110.52
4	B	608	DXC	O1-C13-C12	-3.16	105.68	111.02
4	B	601	DXC	O1-C13-C12	-3.00	105.95	111.02
4	B	608	DXC	C4-C10-C9	2.98	115.46	112.43
4	A	408	DXC	C10-C14-C13	-2.96	110.42	114.29
4	A	407	DXC	C5-C6-C1	2.88	114.30	110.48
4	A	404	DXC	O1-C13-C14	2.80	114.83	109.12
4	B	601	DXC	C20-C12-C17	-2.78	106.84	111.20
4	B	602	DXC	C11-C9-C10	-2.76	105.48	109.09
4	B	601	DXC	C2-C1-C6	2.74	113.96	110.62
4	B	607	DXC	C18-C4-C5	-2.74	103.95	108.31
4	B	601	DXC	C10-C14-C13	-2.64	110.85	114.29
4	A	407	DXC	C4-C10-C9	-2.58	109.81	112.43
4	B	601	DXC	C5-C4-C10	2.57	115.33	111.34
4	B	607	DXC	O1-C13-C12	-2.55	106.71	111.02
4	A	405	DXC	O1-C13-C14	2.54	114.28	109.12
4	B	601	DXC	C5-C4-C3	-2.47	104.20	107.75
4	A	405	DXC	C2-C1-C6	2.47	113.63	110.62
4	A	405	DXC	C22-C21-C19	2.42	118.98	114.46
4	A	406	DXC	O1-C13-C12	-2.40	106.96	111.02
3	B	605	3PE	O12-P-O14	2.39	123.59	112.44
3	A	403	3PE	C2-O21-C21	2.38	123.49	117.80
4	B	608	DXC	C12-C11-C9	-2.34	112.17	114.69
4	A	405	DXC	C3-C2-C1	2.34	116.23	112.71
4	B	602	DXC	C14-C13-C12	2.33	113.63	111.26
4	B	602	DXC	O1-C13-C12	-2.32	107.10	111.02
4	A	406	DXC	C16-C15-C11	-2.31	100.62	105.14
4	B	607	DXC	C21-C19-C17	-2.30	105.56	110.33
5	A	409	PLP	C3-C2-N1	2.29	123.84	120.96
4	B	602	DXC	C12-C17-C19	2.29	122.25	119.48
4	A	405	DXC	C20-C12-C11	-2.26	107.66	111.20
4	B	607	DXC	C2-C1-C6	2.24	113.35	110.62
5	A	409	PLP	C5-C6-N1	-2.23	120.20	123.83
3	A	403	3PE	O12-P-O14	2.23	122.83	112.44
4	A	408	DXC	O3-C23-C22	-2.22	116.05	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	DXC	C15-C11-C12	-2.21	101.39	103.54
4	B	607	DXC	C11-C9-C10	-2.18	106.23	109.09
4	B	608	DXC	C18-C4-C5	-2.18	104.84	108.31
4	B	601	DXC	C20-C12-C13	2.15	111.21	109.06
4	A	408	DXC	C20-C12-C17	-2.15	107.84	111.20
4	A	408	DXC	C20-C12-C13	-2.12	106.94	109.06
4	A	405	DXC	C5-C6-C1	2.12	113.28	110.48
3	B	605	3PE	O21-C2-C1	2.11	115.91	108.34
4	B	602	DXC	C3-C2-C1	-2.11	109.53	112.71
4	B	607	DXC	C2-C3-C7	-2.10	108.09	111.73
4	B	601	DXC	C15-C11-C12	-2.09	101.51	103.54
4	B	606	DXC	C24-C19-C17	-2.09	109.75	112.88
4	A	406	DXC	C2-C3-C7	-2.08	108.13	111.73
4	B	607	DXC	C20-C12-C13	2.07	111.13	109.06
4	A	406	DXC	C18-C4-C10	2.07	113.95	111.18
4	A	404	DXC	C21-C22-C23	2.05	117.95	112.49
4	A	408	DXC	C2-C1-C6	2.05	113.12	110.62
4	B	602	DXC	C10-C14-C13	2.02	116.94	114.29
4	A	407	DXC	O1-C13-C14	2.02	113.22	109.12
4	B	601	DXC	C6-C5-C4	2.00	116.12	112.74

There are no chirality outliers.

All (70) 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	C1-O11-P-O14
3	A	403	3PE	C11-O13-P-O12
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
3	B	605	3PE	C32-C31-O31-C3
4	A	405	DXC	C24-C19-C21-C22
4	B	607	DXC	C24-C19-C21-C22
4	B	608	DXC	C24-C19-C21-C22
3	A	403	3PE	C32-C31-O31-C3
3	A	403	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
3	B	605	3PE	O32-C31-O31-C3
4	A	408	DXC	C24-C19-C21-C22
4	B	608	DXC	C17-C19-C21-C22
4	A	406	DXC	C17-C19-C21-C22
4	A	405	DXC	C17-C19-C21-C22
4	A	406	DXC	C24-C19-C21-C22
4	B	607	DXC	C17-C19-C21-C22
4	A	404	DXC	C24-C19-C21-C22
3	B	605	3PE	C25-C26-C27-C28
3	A	403	3PE	C25-C26-C27-C28
3	A	403	3PE	C3A-C3B-C3C-C3D
3	B	605	3PE	C3A-C3B-C3C-C3D
4	B	606	DXC	C12-C17-C19-C21
4	B	606	DXC	C24-C19-C21-C22
3	B	605	3PE	C26-C27-C28-C29
4	A	406	DXC	C19-C21-C22-C23
4	B	606	DXC	C16-C17-C19-C24
4	B	606	DXC	C12-C17-C19-C24
3	B	605	3PE	O11-C1-C2-O21
3	B	605	3PE	C23-C24-C25-C26
3	A	403	3PE	C2A-C2B-C2C-C2D
3	B	605	3PE	C2B-C2C-C2D-C2E
3	A	403	3PE	C2B-C2C-C2D-C2E
4	B	606	DXC	C16-C17-C19-C21
3	B	605	3PE	C2A-C2B-C2C-C2D
3	B	605	3PE	O11-C1-C2-C3
3	A	403	3PE	O11-C1-C2-C3
3	A	403	3PE	O11-C1-C2-O21
3	A	403	3PE	C11-O13-P-O11
3	A	403	3PE	C11-O13-P-O14
3	B	605	3PE	C11-O13-P-O11
3	A	403	3PE	C21-C22-C23-C24
3	A	403	3PE	C29-C2A-C2B-C2C
4	B	602	DXC	C19-C21-C22-C23
3	B	605	3PE	C29-C2A-C2B-C2C
3	B	605	3PE	C21-C22-C23-C24
4	A	408	DXC	C21-C22-C23-O4
4	A	408	DXC	C21-C22-C23-O3
4	A	406	DXC	C21-C22-C23-O3
4	B	606	DXC	C21-C22-C23-O3
4	A	406	DXC	C12-C17-C19-C24
4	A	405	DXC	C12-C17-C19-C21

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Mol	Chain	Res	Type	Atoms
3	B	605	3PE	C39-C3A-C3B-C3C
4	B	606	DXC	C21-C22-C23-O4
4	A	408	DXC	C19-C21-C22-C23
3	A	403	3PE	C39-C3A-C3B-C3C
3	B	605	3PE	C32-C33-C34-C35
3	B	605	3PE	C28-C29-C2A-C2B
4	A	404	DXC	C21-C22-C23-O3
4	B	602	DXC	C16-C17-C19-C21
4	A	406	DXC	C21-C22-C23-O4
4	A	404	DXC	C21-C22-C23-O4
4	A	406	DXC	C16-C17-C19-C21

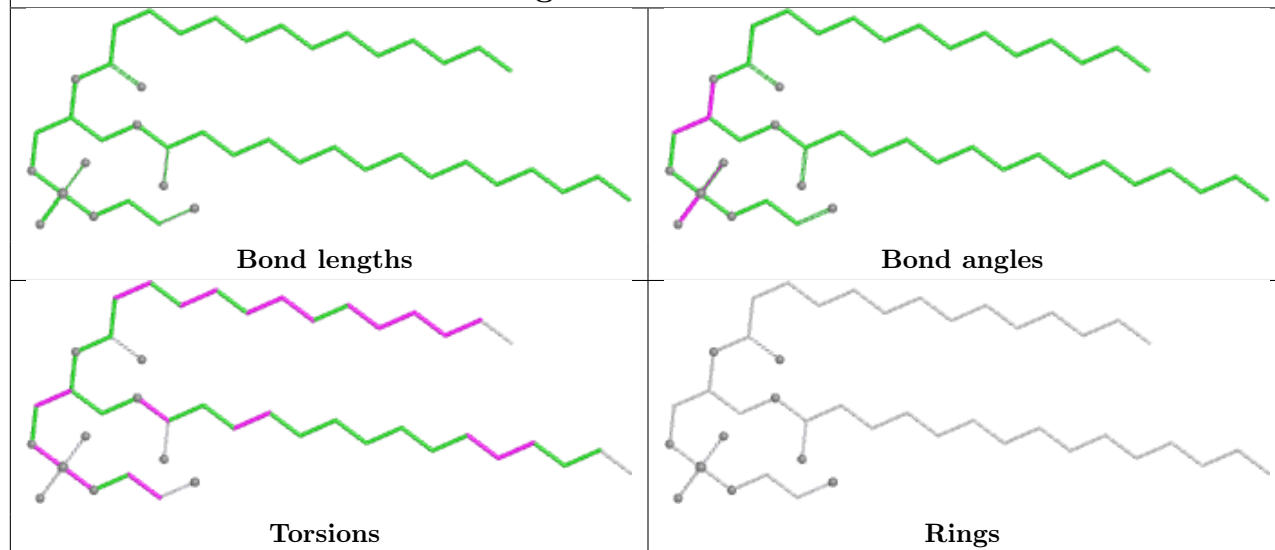
There are no ring outliers.

12 monomers are involved in 27 short contacts:

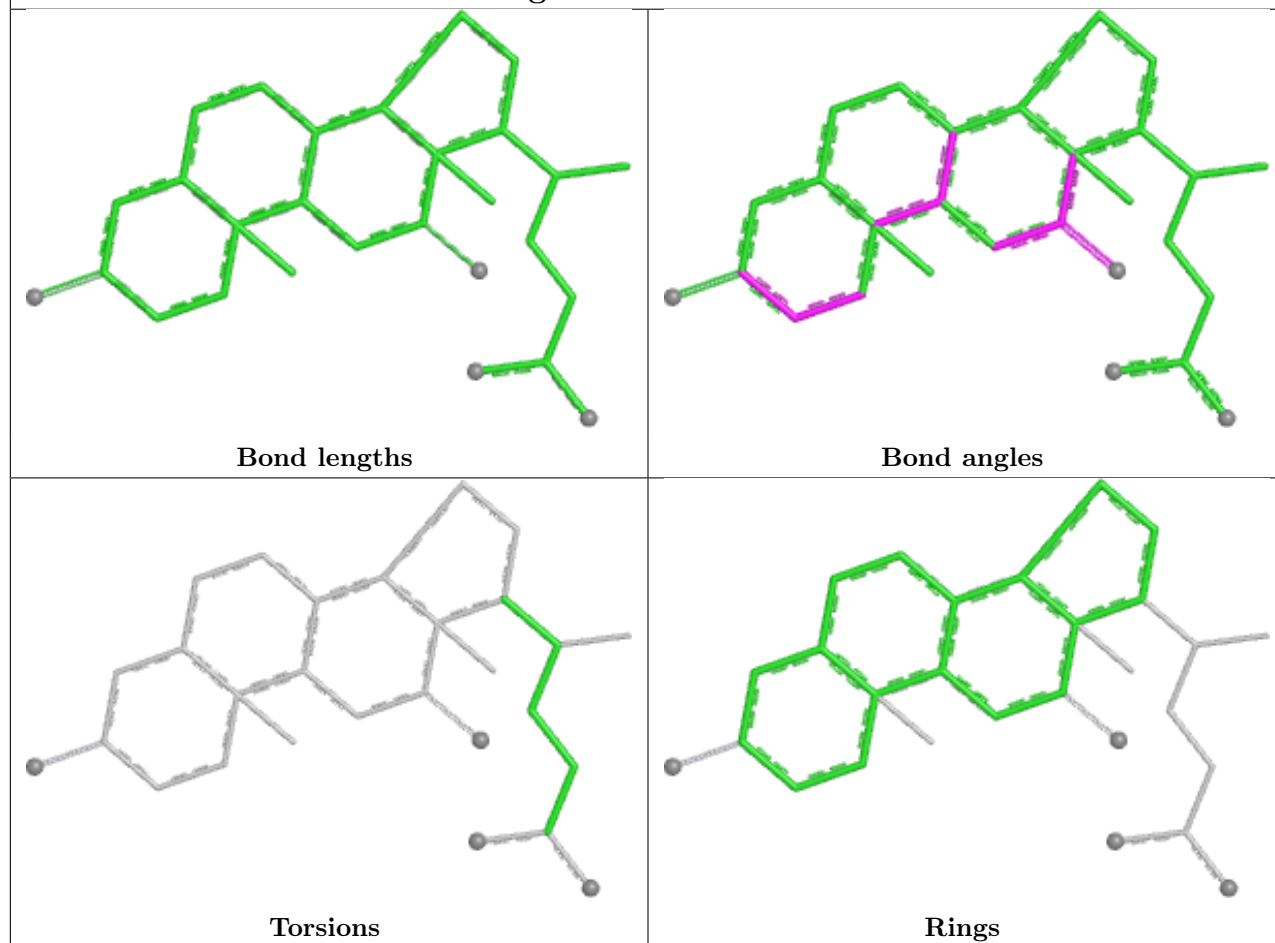
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	605	3PE	3	0
4	A	407	DXC	1	0
5	A	409	PLP	2	0
4	B	608	DXC	2	0
4	A	408	DXC	5	0
3	A	403	3PE	6	0
4	A	405	DXC	3	0
4	B	601	DXC	1	0
4	B	607	DXC	2	0
4	B	602	DXC	4	0
4	A	404	DXC	2	0
4	A	406	DXC	3	0

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

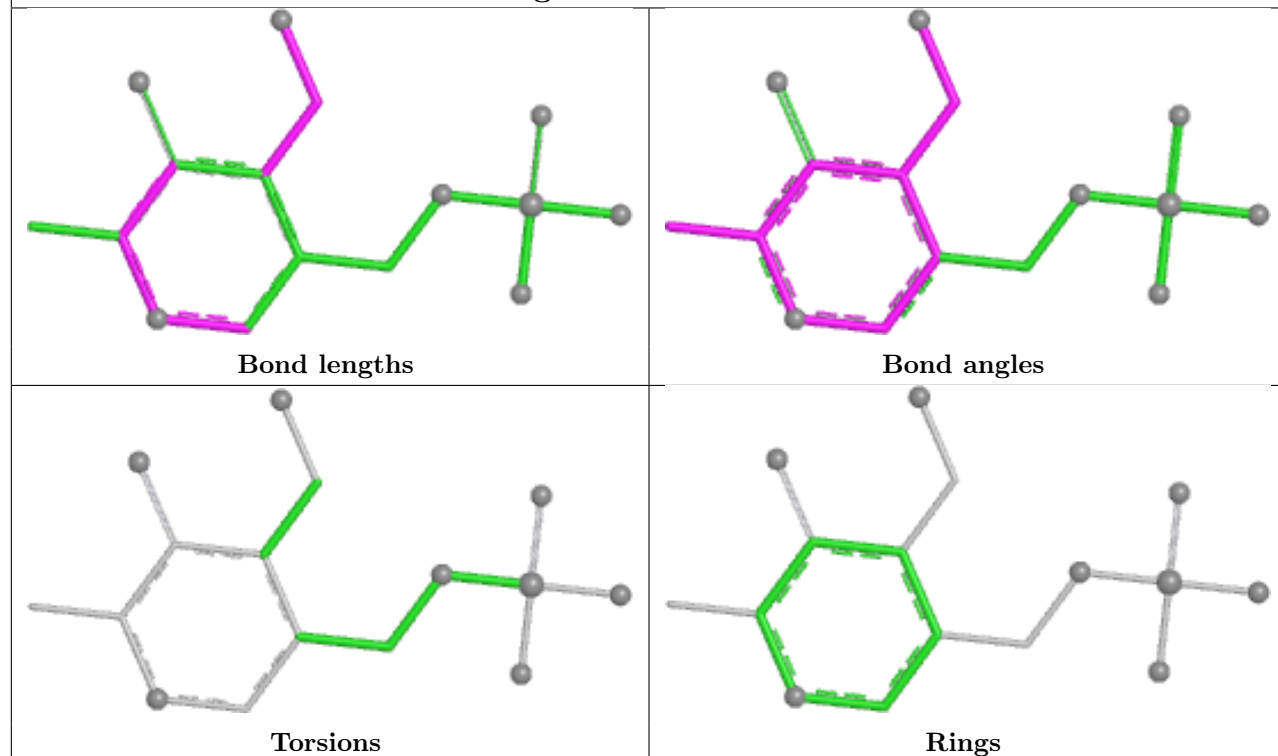
Ligand 3PE B 605



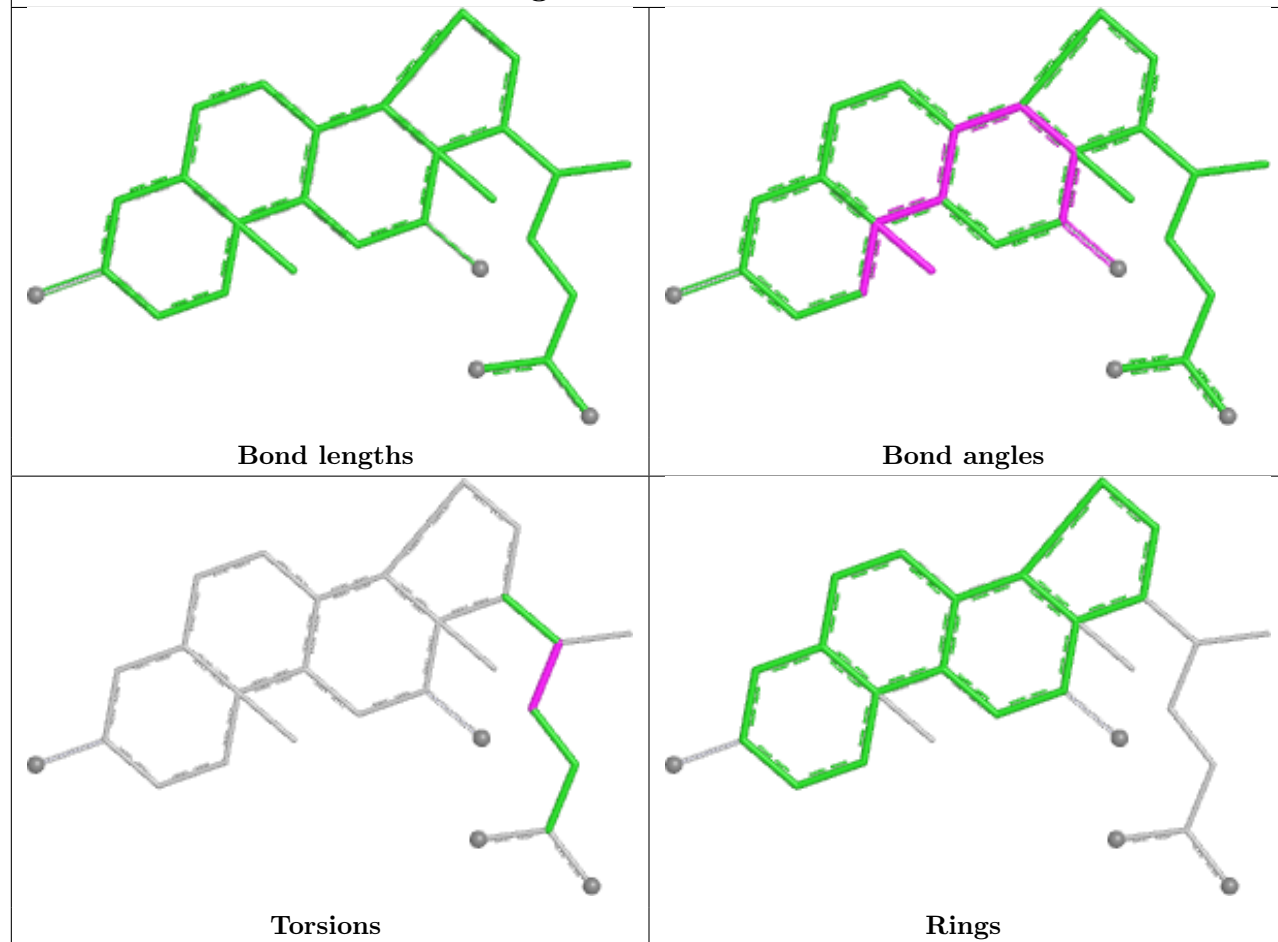
Ligand DXC A 407

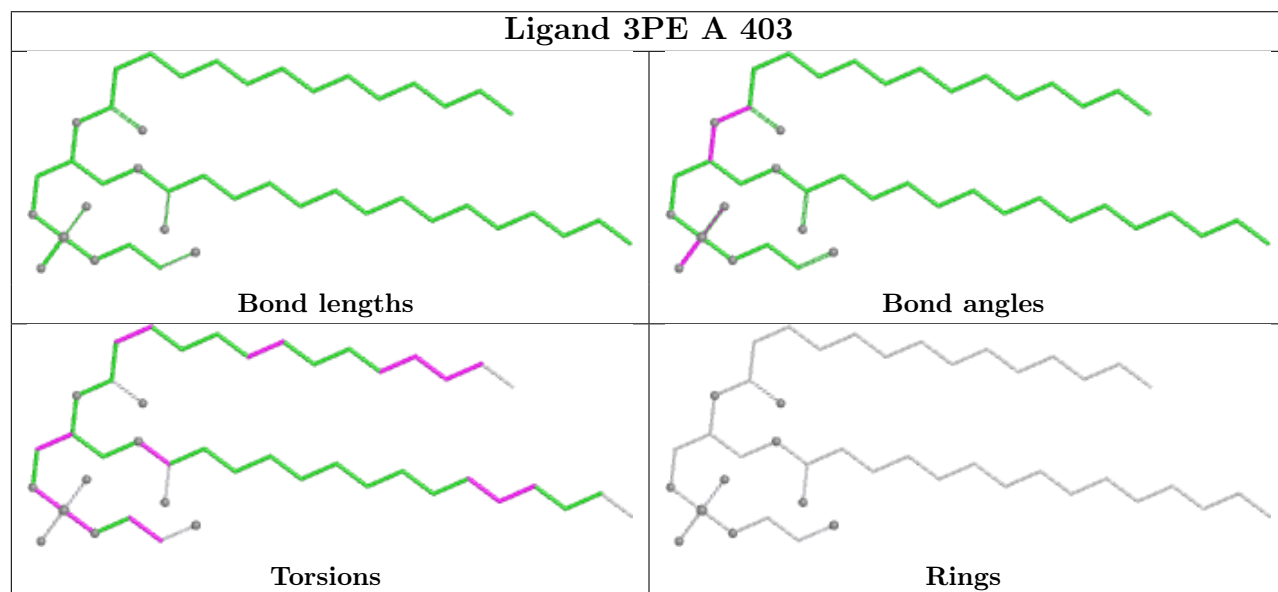
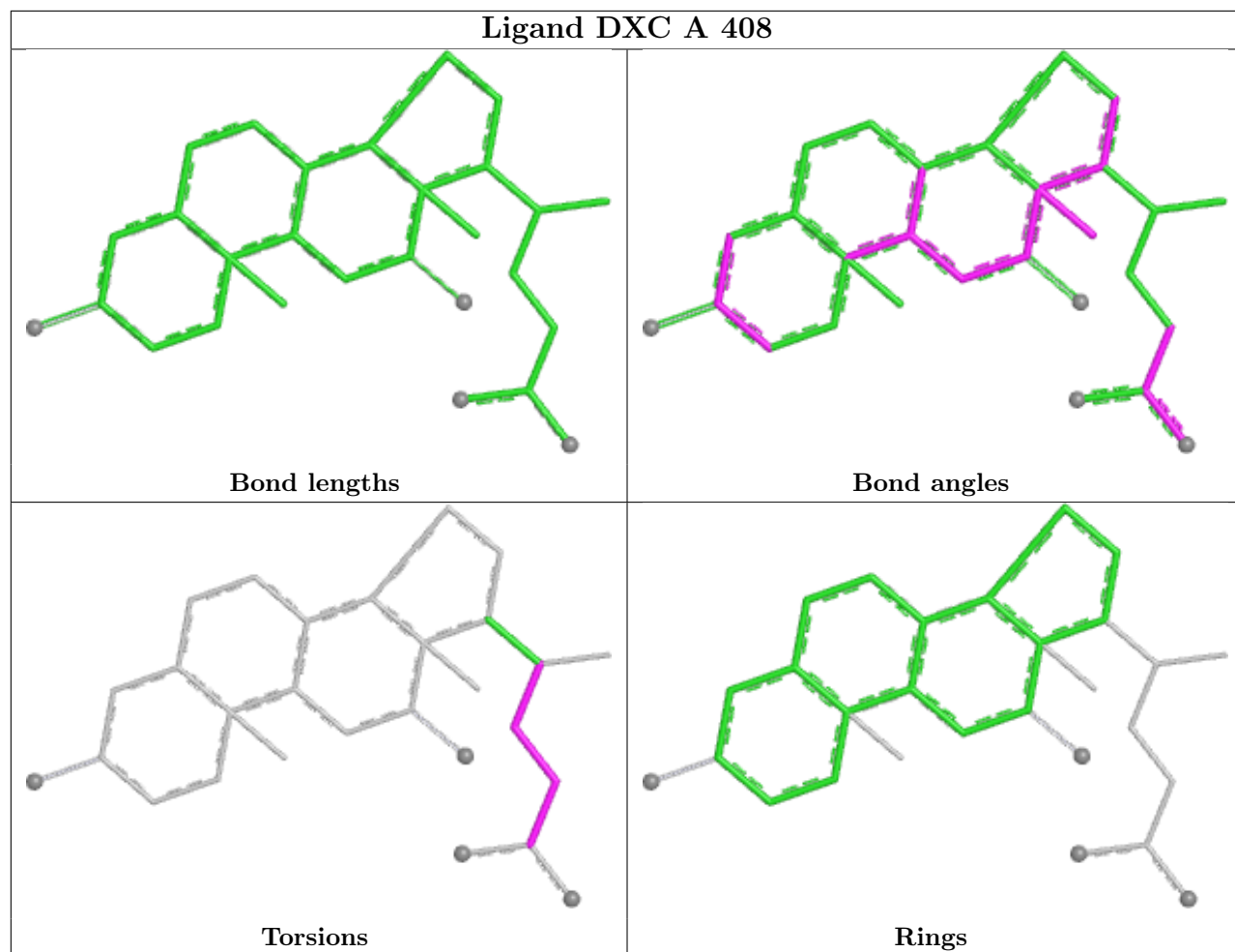


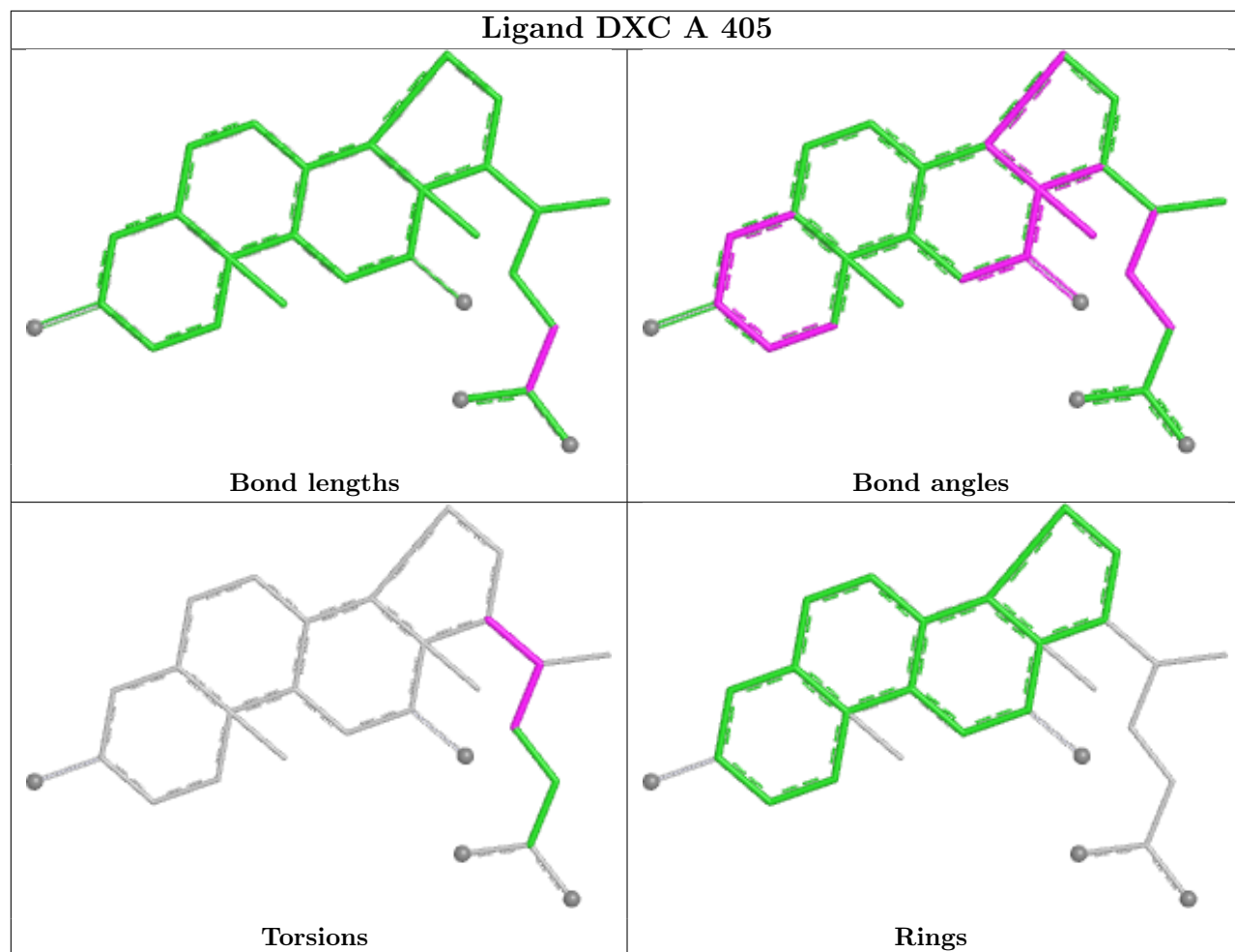
Ligand PLP A 409

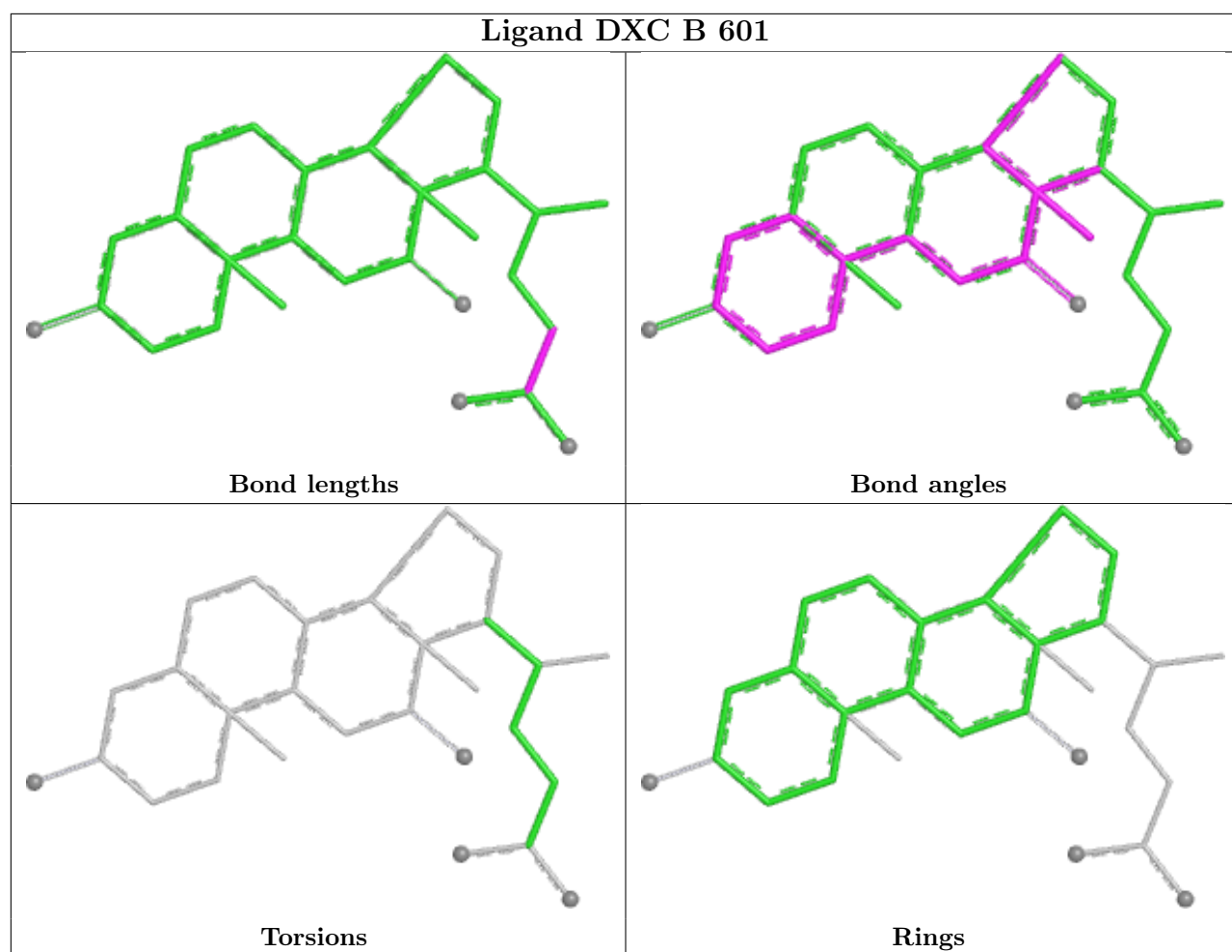


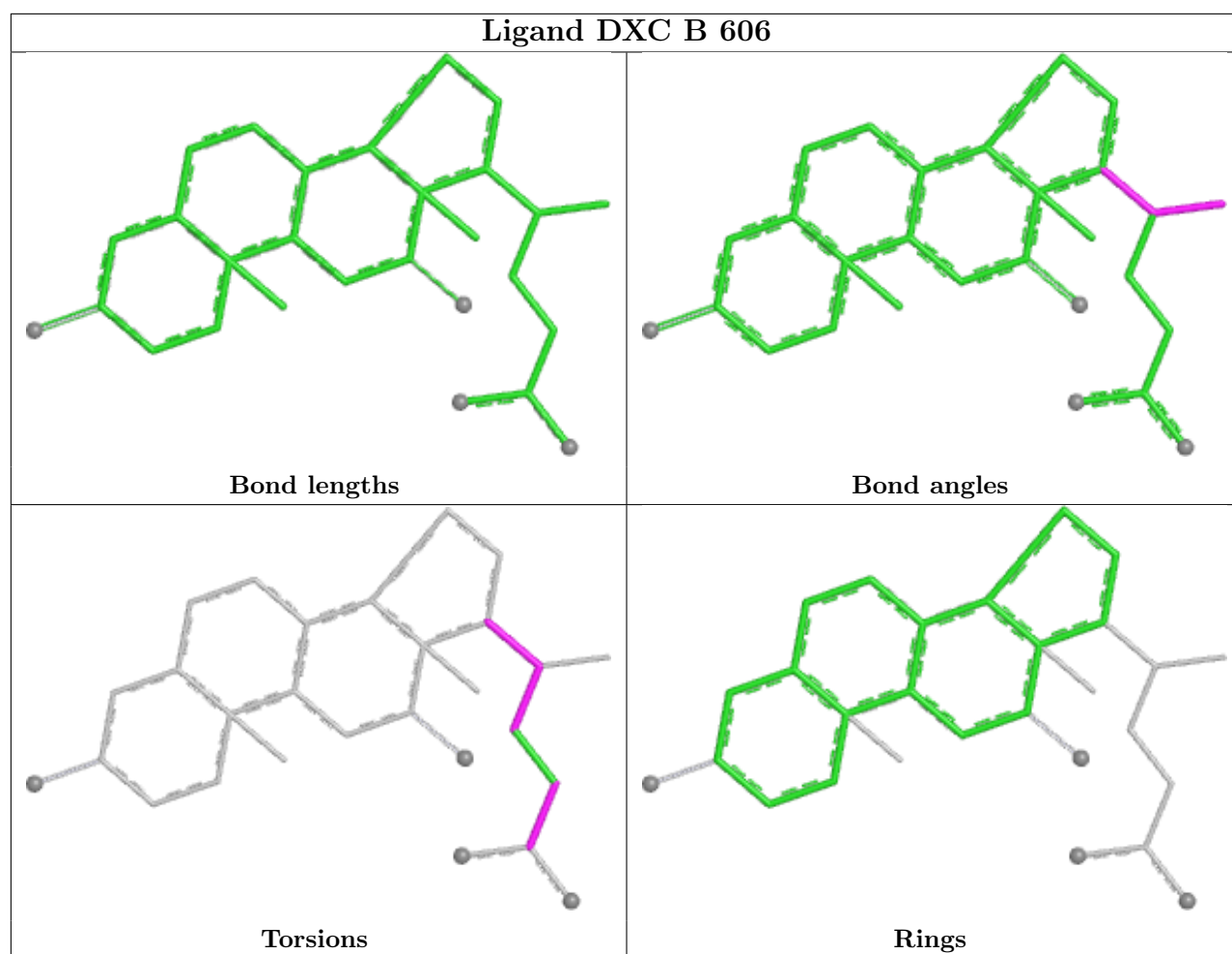
Ligand DXC B 608

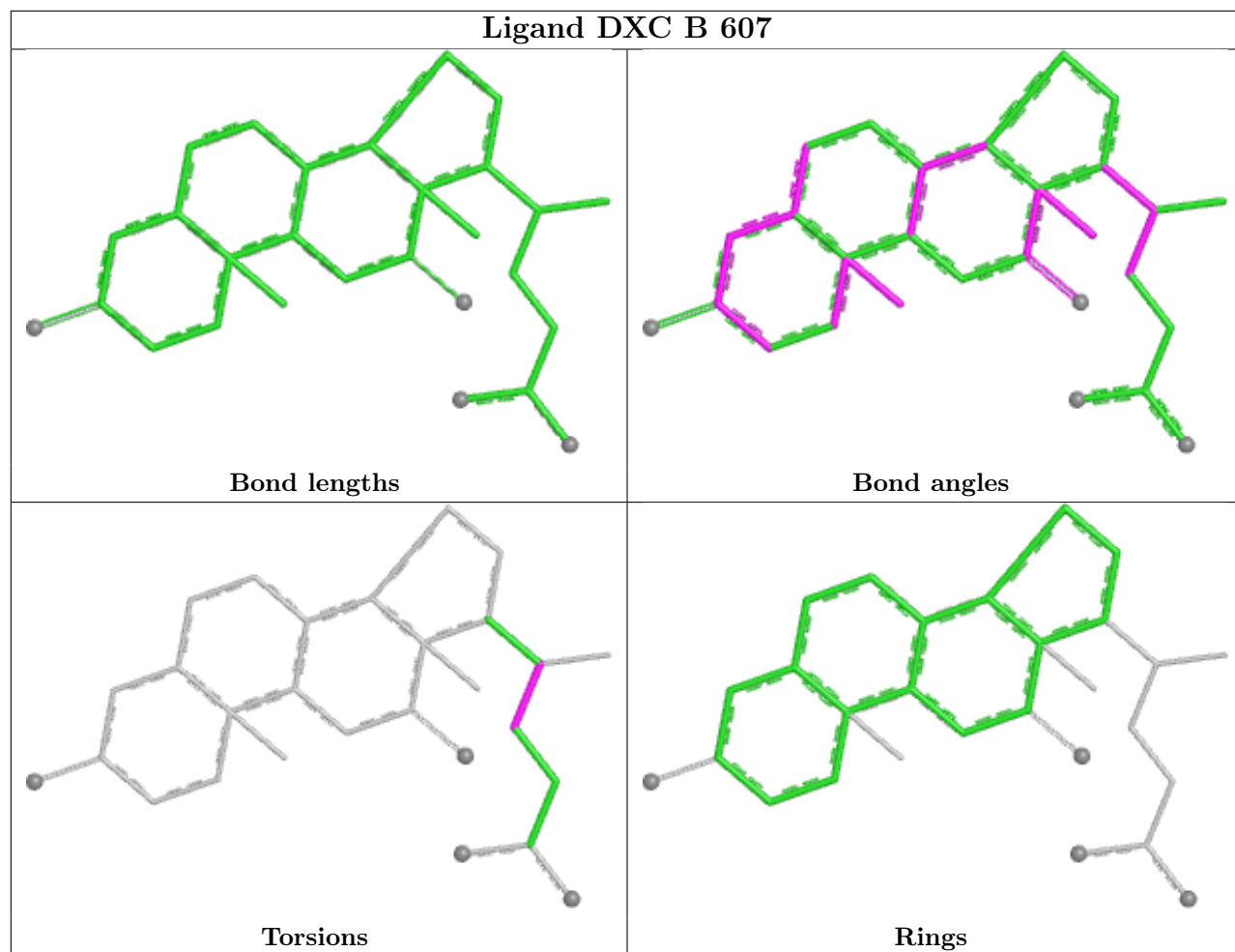


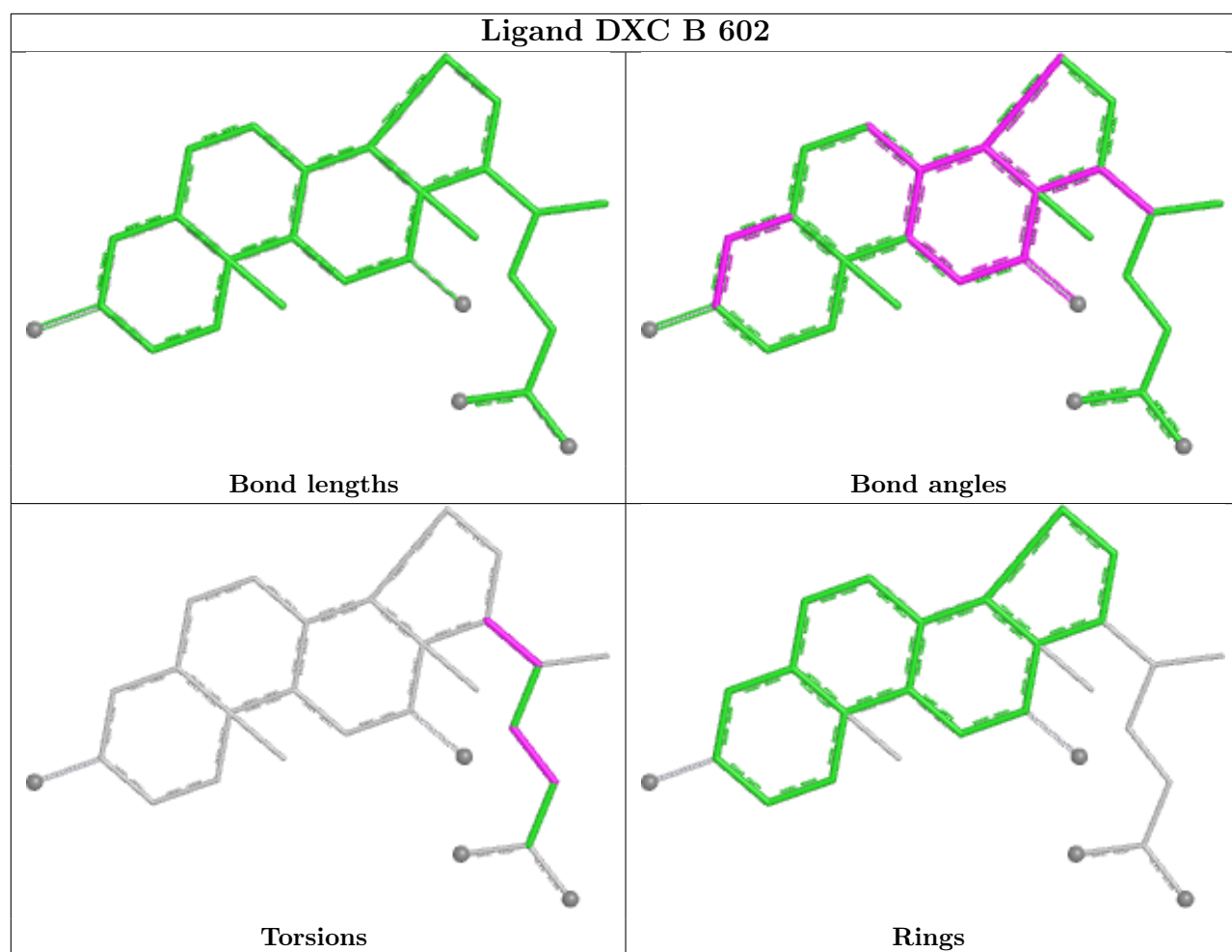


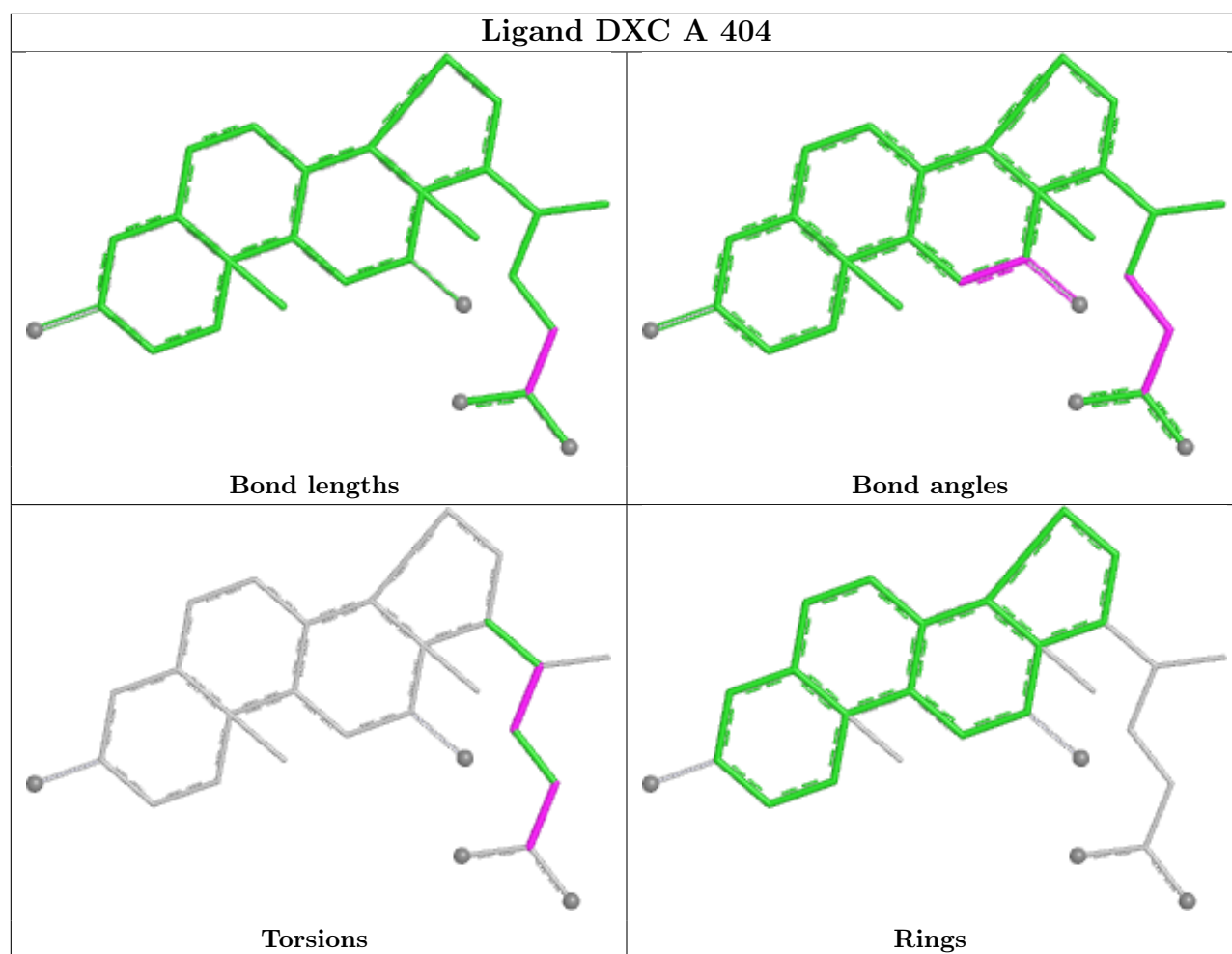


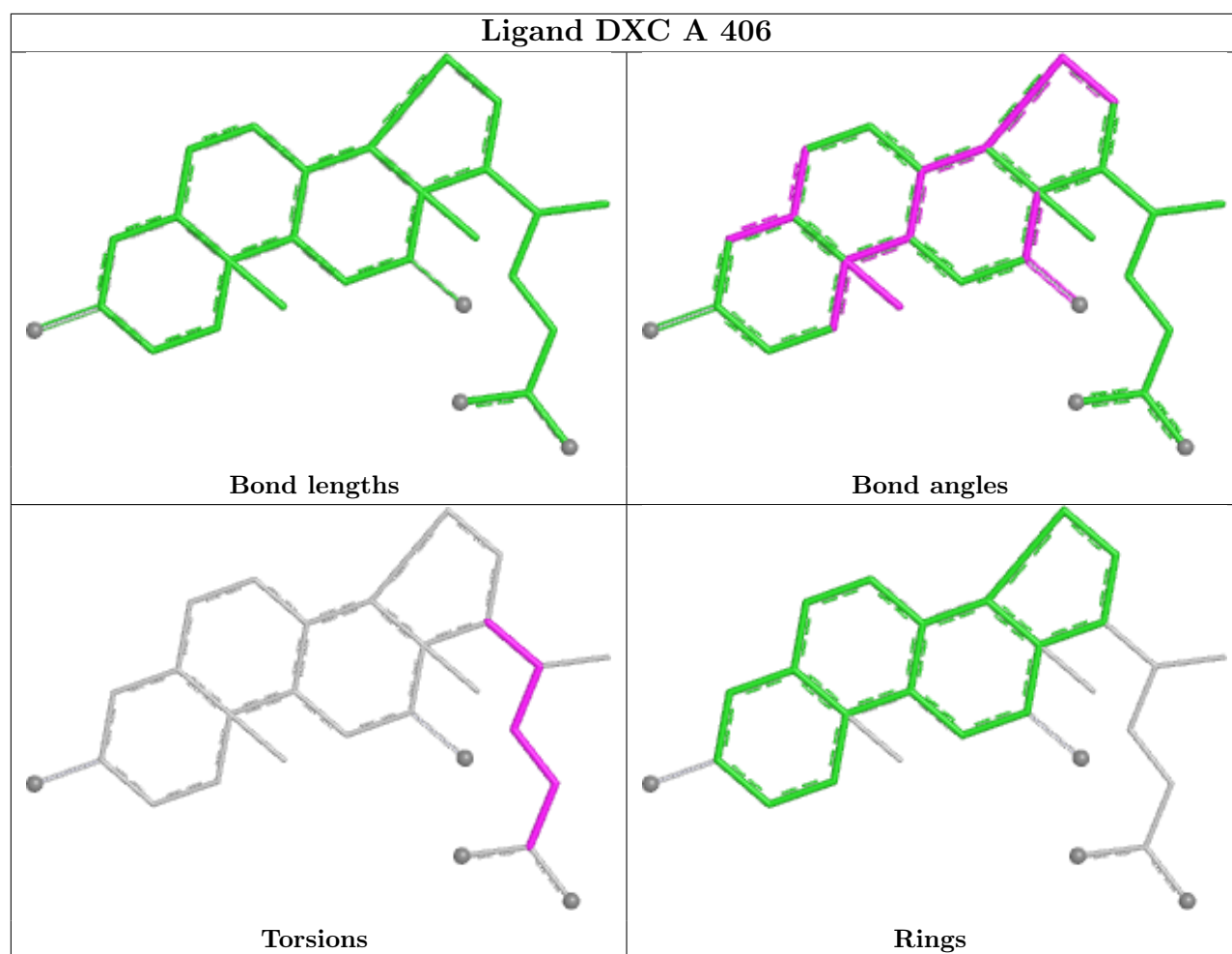












5.7 Other polymers [i](#)

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%)	0.94	39 (11%) 9 7	58, 126, 164, 182	2 (0%)
1	B	334/393 (84%)	0.55	21 (6%) 26 19	60, 102, 158, 198	3 (0%)
All	All	666/786 (84%)	0.75	60 (9%) 15 11	58, 114, 162, 198	5 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	84	LEU	7.2
1	B	72[A]	TRP	6.0
1	B	83	TRP	5.2
1	B	85	ILE	4.6
1	A	83	TRP	4.4
1	A	84	LEU	4.4
1	A	72	TRP	4.2
1	A	73	LYS	4.0
1	B	80	VAL	3.9
1	A	314	ARG	3.8
1	A	69	TRP	3.8
1	A	260	MET	3.8
1	B	73	LYS	3.4
1	B	81	LEU	3.3
1	B	88	LYS	3.3
1	A	166	ARG	3.2
1	A	89	ASP	3.1
1	A	167[A]	ARG	3.1
1	B	65	PHE	3.0
1	A	340	MET	3.0
1	A	95	SER	2.9
1	A	315[A]	TRP	2.9
1	B	116[A]	GLU	2.9
1	B	87	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	89	ASP	2.9
1	A	319	TYR	2.8
1	A	80	VAL	2.8
1	A	313	PRO	2.8
1	A	291	PHE	2.8
1	A	78	PRO	2.7
1	B	86	MET	2.7
1	A	318	LYS	2.6
1	B	94	PRO	2.6
1	A	244	VAL	2.5
1	B	77	ILE	2.5
1	A	246	PHE	2.5
1	A	79	ASN	2.5
1	A	85	ILE	2.5
1	A	232	TRP	2.4
1	A	67	ASN	2.4
1	A	74	ASN	2.4
1	B	335	GLN	2.3
1	A	93	VAL	2.3
1	A	179	ASP	2.3
1	A	251	SER	2.3
1	A	66	VAL	2.3
1	A	273	LEU	2.2
1	B	67	ASN	2.2
1	A	71	THR	2.2
1	A	81	LEU	2.2
1	A	90	HIS	2.1
1	A	259	LEU	2.1
1	B	206	GLU	2.1
1	B	74	ASN	2.1
1	A	145	LEU	2.1
1	A	309	GLY	2.1
1	B	317	MET	2.0
1	B	319	TYR	2.0
1	A	132	HIS	2.0
1	A	143	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

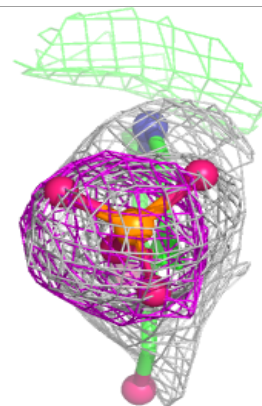
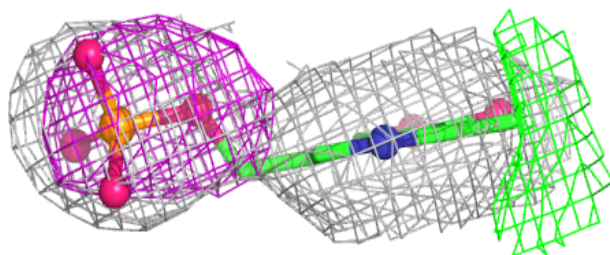
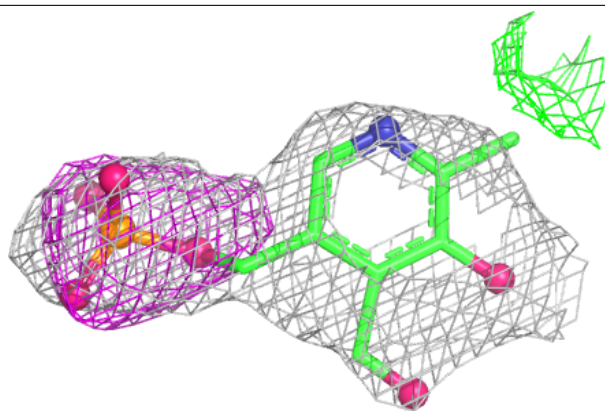
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PLP	A	409	16/16	0.66	0.19	128,128,129,129	0
4	DXC	B	608	28/28	0.82	0.19	123,129,142,148	0
4	DXC	A	408	28/28	0.83	0.17	124,139,159,163	0
4	DXC	A	406	28/28	0.90	0.23	104,110,119,122	28
4	DXC	A	404	28/28	0.92	0.13	95,104,127,130	0
4	DXC	B	601	28/28	0.94	0.14	86,96,102,103	0
4	DXC	B	602	28/28	0.94	0.14	92,95,98,100	28
4	DXC	B	607	28/28	0.94	0.15	100,104,126,135	0
3	3PE	A	403	44/51	0.94	0.16	92,106,112,117	0
4	DXC	A	405	28/28	0.94	0.12	92,99,113,117	0
4	DXC	B	606	28/28	0.95	0.11	87,92,112,116	0
3	3PE	B	605	44/51	0.95	0.14	97,105,116,121	0
4	DXC	A	407	28/28	0.96	0.14	93,100,106,111	0
2	ZN	B	603	1/1	0.99	0.06	88,88,88,88	0
2	ZN	B	604	1/1	0.99	0.03	89,89,89,89	0
2	ZN	A	402	1/1	0.99	0.05	110,110,110,110	0
2	ZN	A	401	1/1	1.00	0.05	97,97,97,97	0

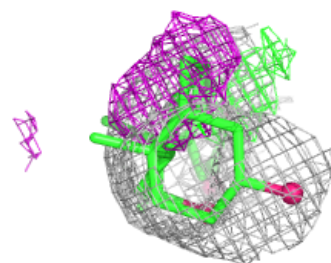
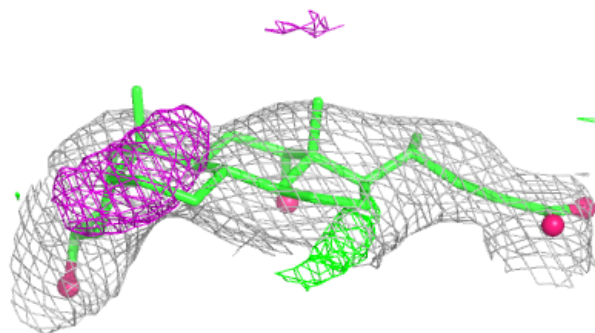
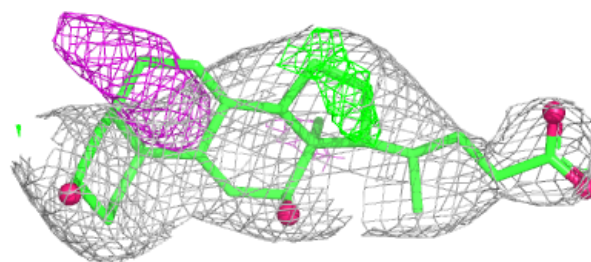
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PLP 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)

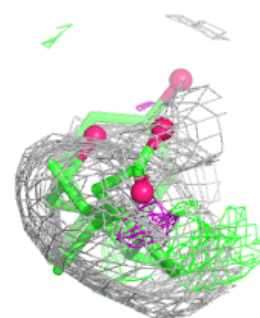
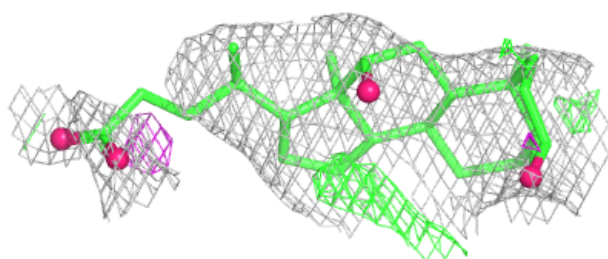
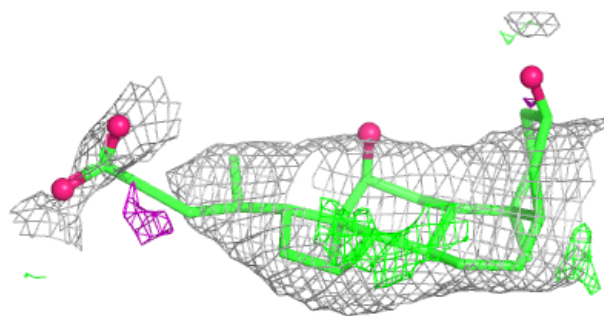
**Electron density around DXC B 608:**

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

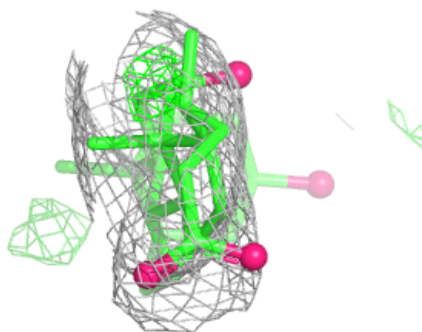
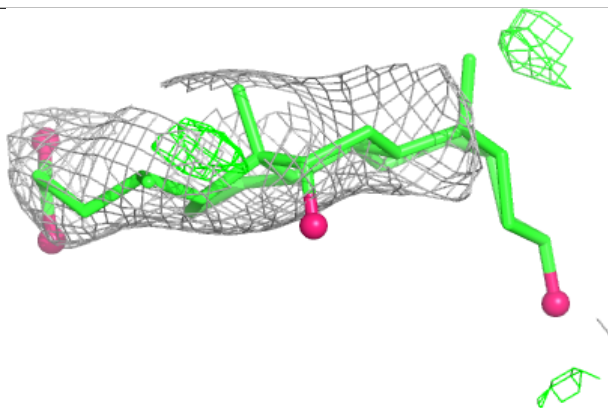
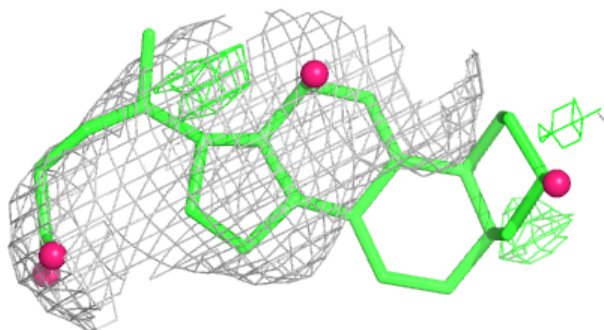


Electron density around DXC A 408:

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

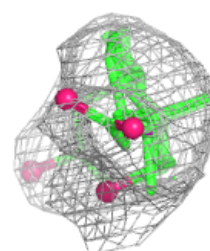
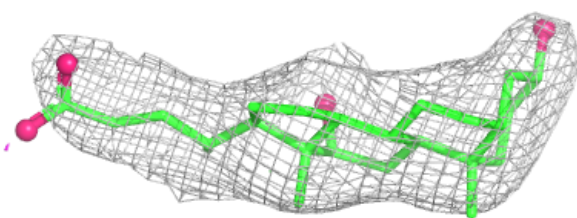
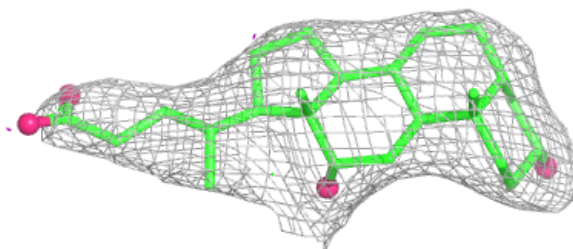
**Electron density around DXC A 406:**

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

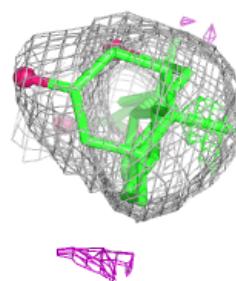
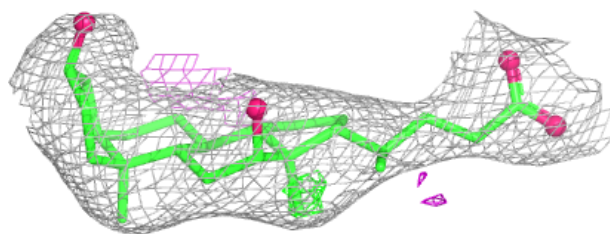
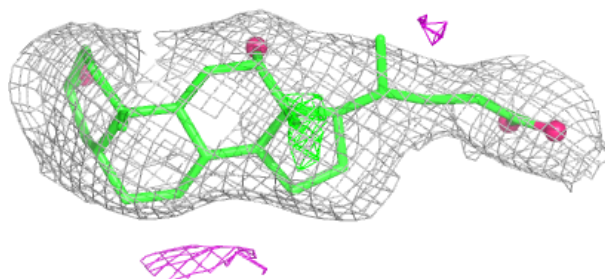


Electron density around DXC A 404:

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

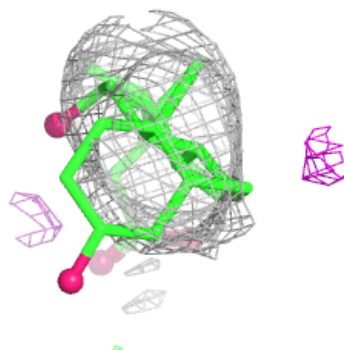
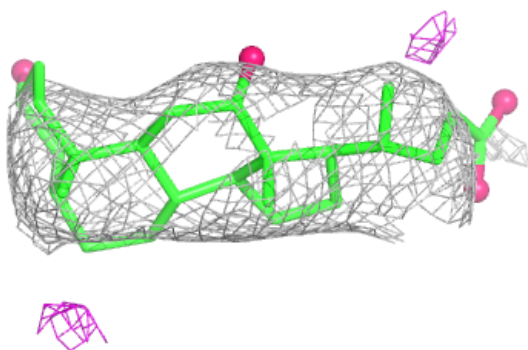
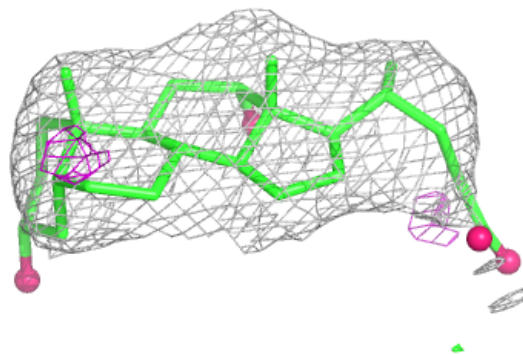
**Electron density around DXC B 601:**

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

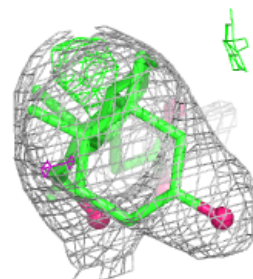
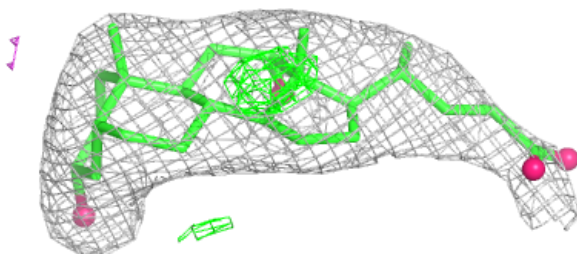
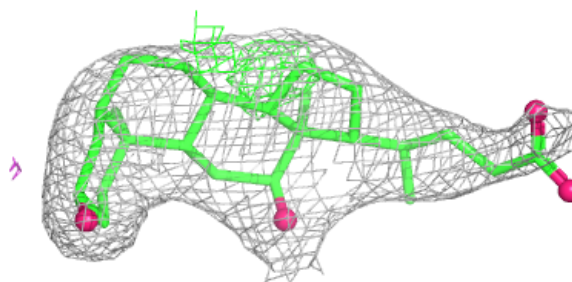


Electron density around DXC B 602:

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

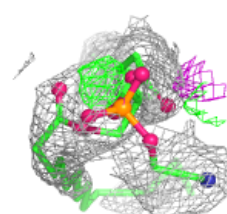
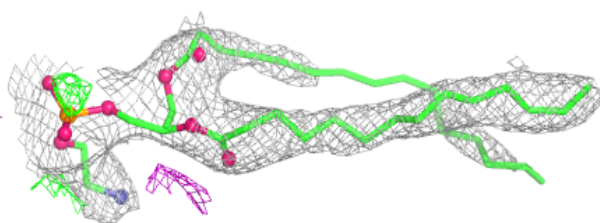
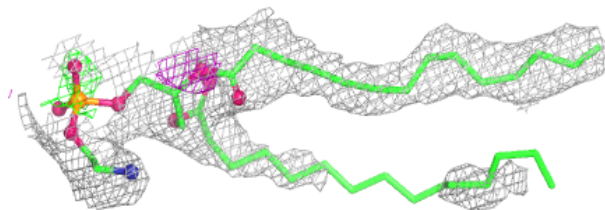
**Electron density around DXC B 607:**

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

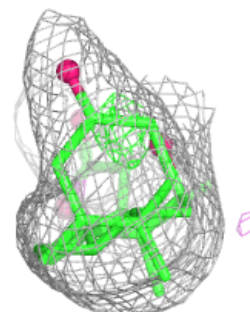
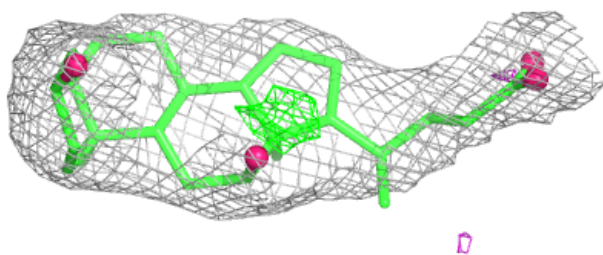
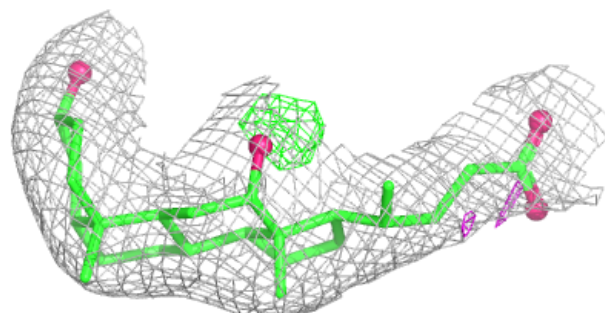


Electron density around 3PE A 403:

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

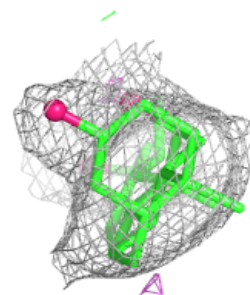
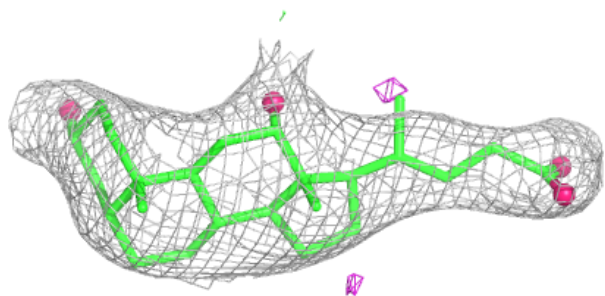
**Electron density around DXC A 405:**

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

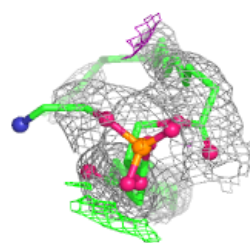
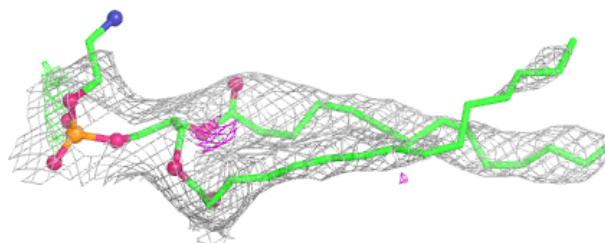
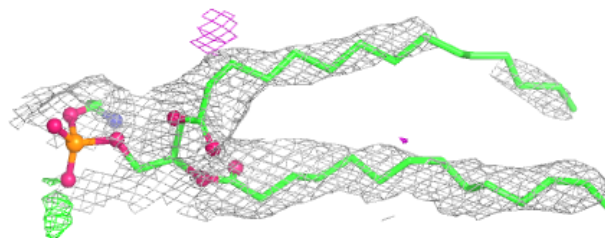


Electron density around DXC B 606:

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

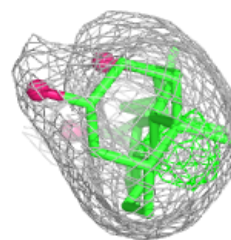
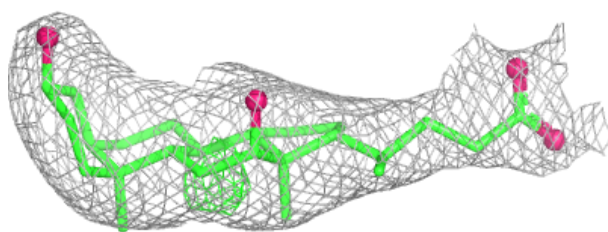
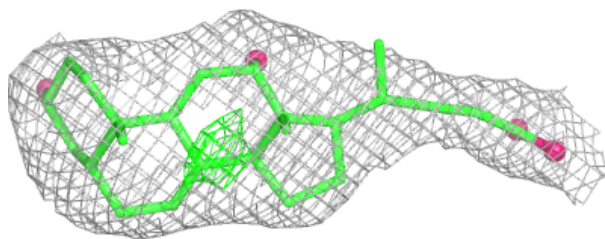
**Electron density around 3PE B 605:**

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



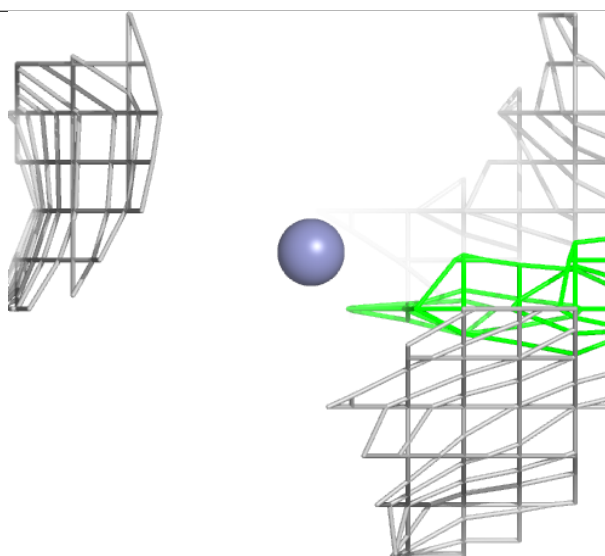
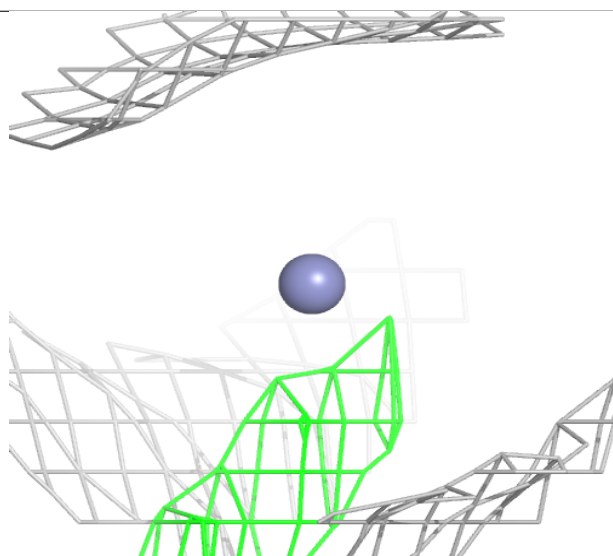
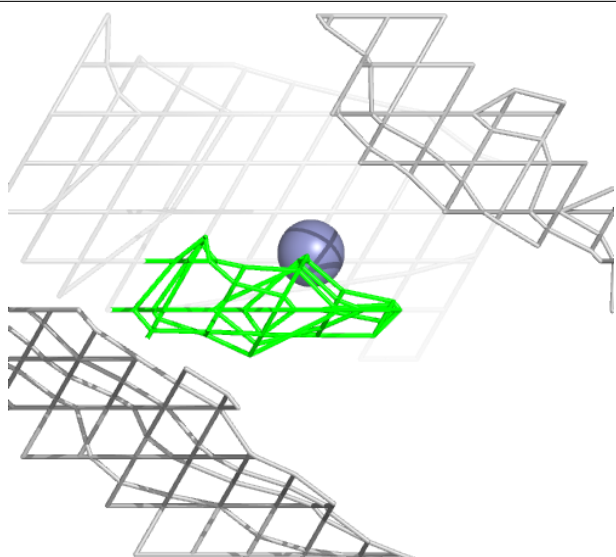
Electron density around DXC A 407:

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



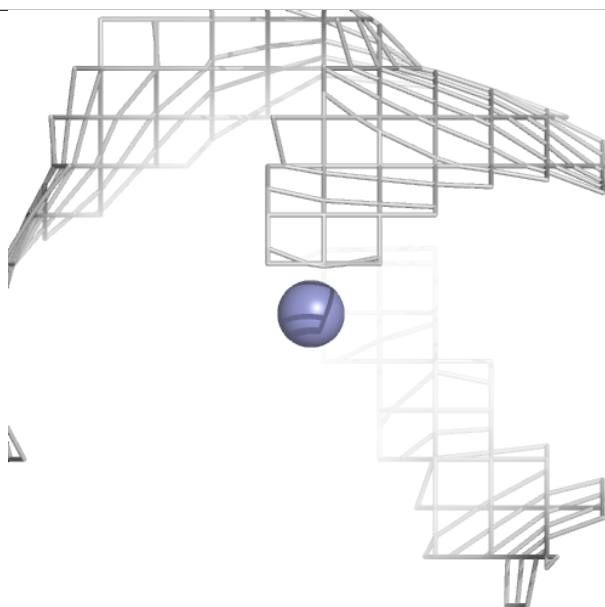
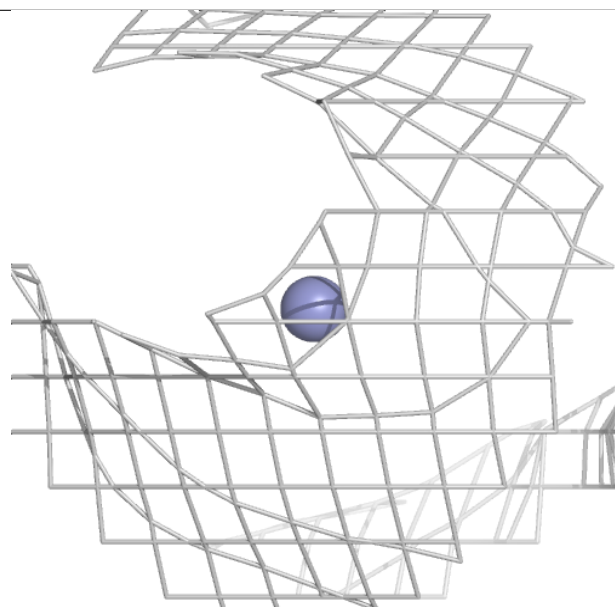
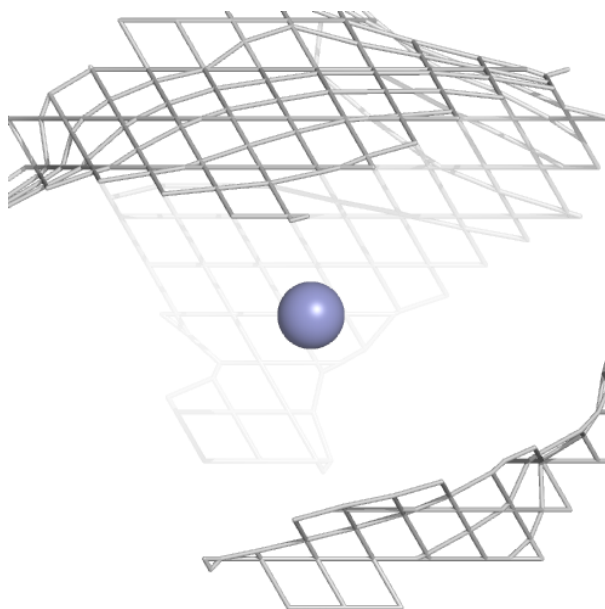
Electron density around ZN B 603:

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and green (positive)



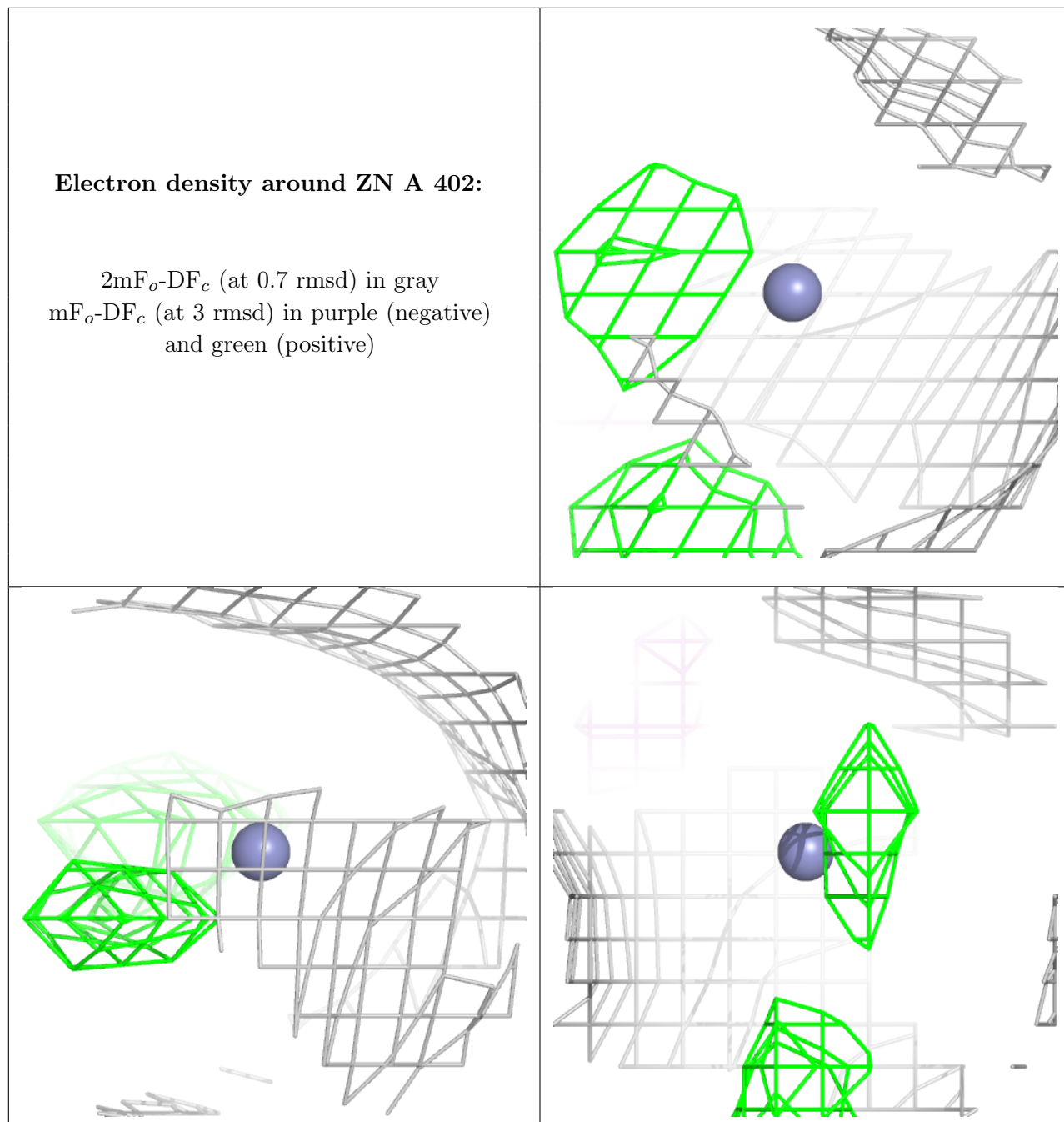
Electron density around ZN B 604:

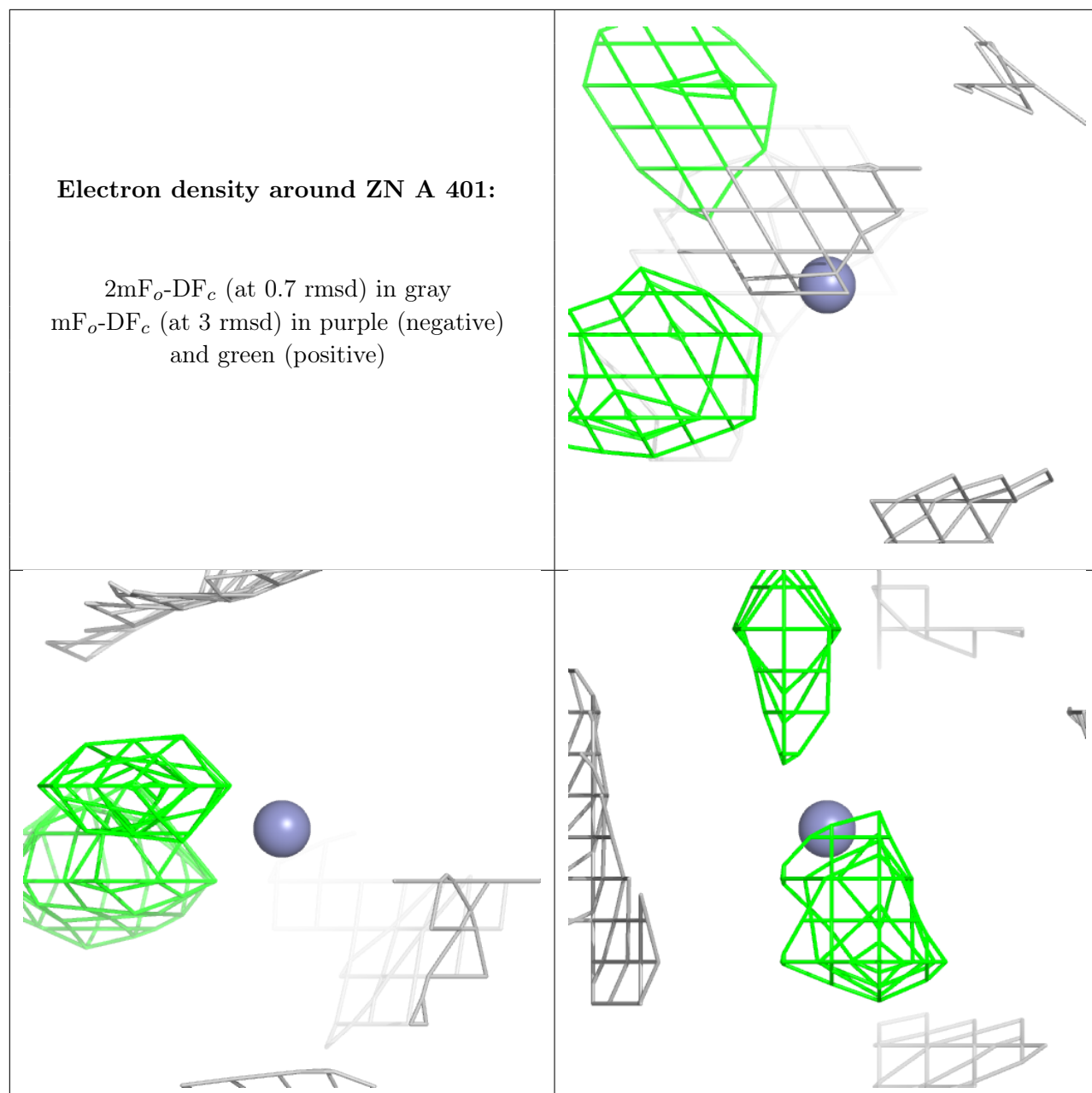
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

There are no such residues in this entry.