



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:53 AM UTC

PDB ID : 4QN9 / pdb_00004qn9
Title : Structure of human NAPE-PLD
Authors : Garau, G.
Deposited on : 2014-06-17
Resolution : 2.65 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

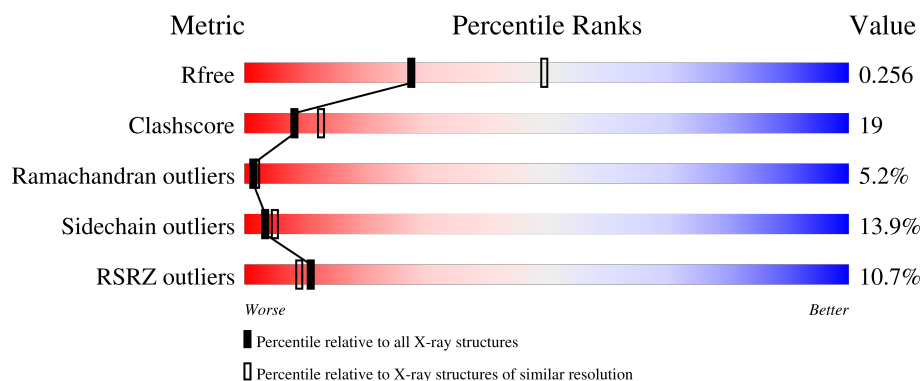
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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% 52% 21% 6% • 18%
1	B	393	7% 51% 21% 7% • 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	B	611	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5875 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.

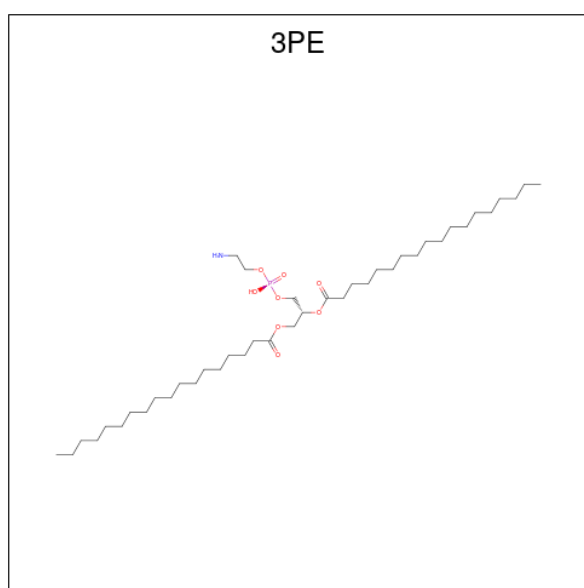
- Molecule 1 is a protein called N-acyl-phosphatidylethanolamine-hydrolyzing phospholipase D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	8	0
			2679	1732	452	482	13			
1	B	322	Total	C	N	O	S	0	7	0
			2682	1732	452	485	13			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

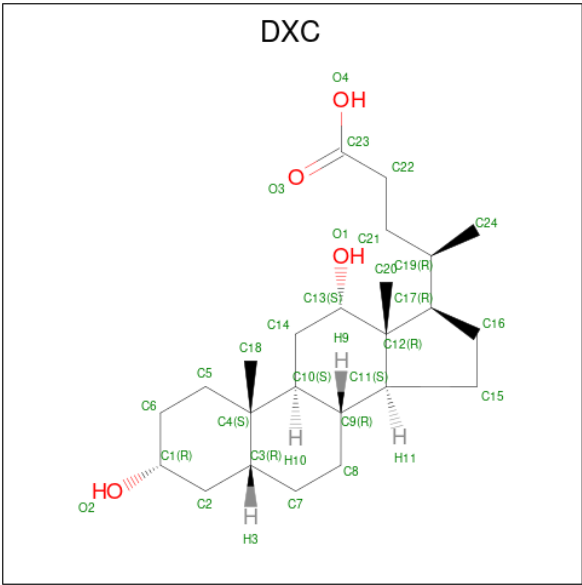
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



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).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

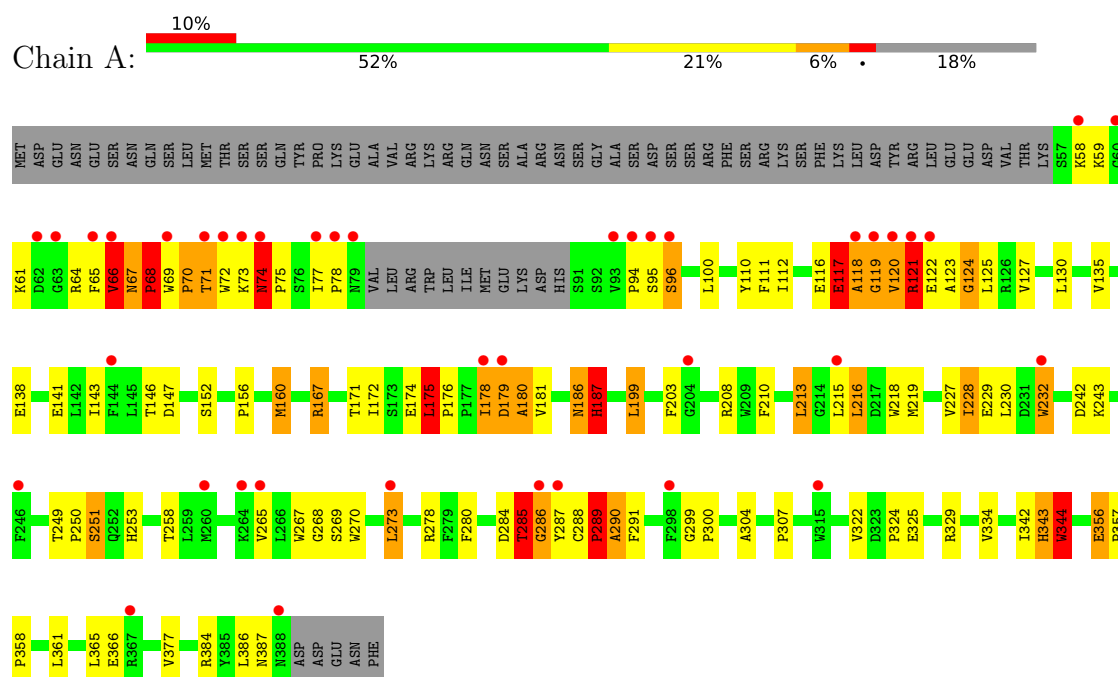
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	0
			36	36		
6	B	62	Total	O	0	1
			63	63		

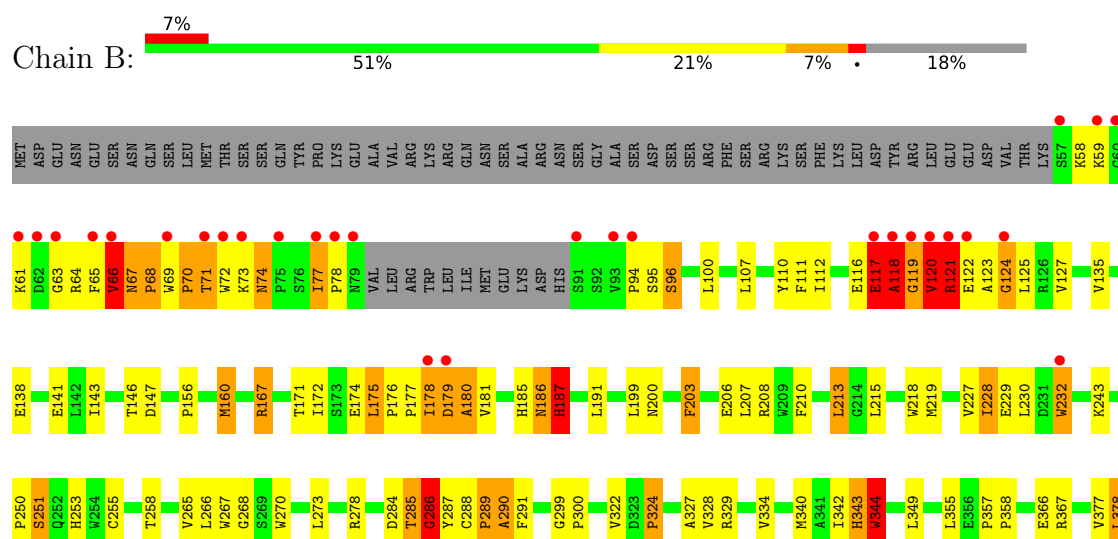
3 Residue-property plots [i](#)

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



R384	N387	N388	D389	ASP	GLU	ASN	PHE
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4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	95.10Å 95.10Å 444.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.36 – 2.65 82.36 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (82.36-2.65) 100.0 (82.36-2.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.65Å)	Xtriage
Refinement program	CCP4, REFMAC 5.7.0029	Depositor
R, R_{free}	0.214 , 0.253 0.218 , 0.256	Depositor DCC
R_{free} test set	1794 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 84.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5875	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: DXC, ZN, SO4, 3PE

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	1/2774 (0.0%)	1.14	16/3777 (0.4%)
1	B	1.06	5/2773 (0.2%)	1.19	12/3777 (0.3%)
All	All	0.96	6/5547 (0.1%)	1.16	28/7554 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	8
All	All	0	17

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	118	ALA	C-O	-7.39	1.17	1.24
1	B	71	THR	CA-C	6.62	1.61	1.52
1	A	71	THR	CA-C	6.54	1.61	1.52
1	B	117	GLU	CA-C	5.87	1.60	1.52
1	B	286	GLY	CA-C	-5.12	1.44	1.51
1	B	344	TRP	N-CA	5.12	1.52	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ARG	NE-CZ-NH2	-11.36	108.98	119.20
1	A	121	ARG	CD-NE-CZ	10.27	138.77	124.40
1	A	287	TYR	N-CA-C	-10.17	92.67	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ARG	NE-CZ-NH1	-9.40	112.10	121.50
1	B	121	ARG	NE-CZ-NH2	8.99	127.29	119.20
1	B	287	TYR	N-CA-C	-8.68	95.09	109.24
1	A	285	THR	O-C-N	-7.25	115.64	123.26
1	B	232	TRP	CA-CB-CG	7.17	127.21	113.60
1	B	203	PHE	N-CA-C	-6.85	100.65	110.59
1	A	232	TRP	CA-CB-CG	6.85	126.61	113.60
1	A	203	PHE	N-CA-C	-6.77	100.44	110.46
1	B	121	ARG	CD-NE-CZ	6.63	133.69	124.40
1	B	117	GLU	N-CA-C	6.38	124.39	110.80
1	A	186	ASN	N-CA-C	-6.13	100.23	109.79
1	B	344	TRP	N-CA-C	6.07	123.72	110.80
1	A	325	GLU	N-CA-C	-5.75	104.91	111.07
1	A	66	VAL	N-CA-CB	5.75	120.71	111.23
1	B	186	ASN	N-CA-C	-5.65	100.97	109.79
1	A	356	GLU	CA-C-N	-5.38	114.84	120.38
1	A	356	GLU	C-N-CA	-5.38	114.84	120.38
1	A	344	TRP	N-CA-C	5.33	122.15	110.80
1	B	187	HIS	N-CA-CB	5.30	119.44	110.49
1	B	230	LEU	N-CA-C	5.28	118.03	109.06
1	A	230	LEU	N-CA-C	5.25	117.63	108.76
1	B	118	ALA	N-CA-C	-5.23	101.44	108.19
1	A	187	HIS	N-CA-CB	5.22	119.31	110.49
1	A	289	PRO	N-CA-C	-5.07	102.02	112.47
1	A	121	ARG	NE-CZ-NH1	5.00	126.50	121.50

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	GLU	Peptide
1	A	117	GLU	Peptide
1	A	118	ALA	Peptide
1	A	121	ARG	Sidechain
1	A	175[A]	LEU	Peptide
1	A	285	THR	Mainchain,Peptide
1	A	286	GLY	Mainchain,Peptide
1	B	116	GLU	Peptide
1	B	117	GLU	Peptide
1	B	118	ALA	Peptide
1	B	120	VAL	Peptide
1	B	175[A]	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	B	285	THR	Peptide
1	B	286	GLY	Mainchain,Peptide

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	2679	0	2572	99	0
1	B	2682	0	2567	114	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	62	1	0
3	B	44	0	62	1	0
4	A	112	0	156	10	0
4	B	196	0	273	8	0
5	A	10	0	0	1	0
5	B	5	0	0	2	0
6	A	36	0	0	0	0
6	B	63	0	0	3	0
All	All	5875	0	5692	221	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 19.

All (221) 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:118:ALA:HB1	1:B:138:GLU:OE1	1.41	1.17
1:A:118:ALA:HB1	1:A:138:GLU:OE1	1.50	1.10
1:B:175[B]:LEU:HB2	1:B:176[B]:PRO:HD2	1.09	1.07
1:A:232:TRP:HZ3	1:A:267:TRP:O	1.39	1.06
1:B:232:TRP:HZ3	1:B:267:TRP:O	1.39	1.05
1:B:175[B]:LEU:CB	1:B:176[B]:PRO:HD2	1.84	1.03
1:A:175[B]:LEU:CB	1:A:176[B]:PRO:HD2	1.83	1.03
1:A:175[B]:LEU:HD12	1:A:175[B]:LEU:H	1.25	1.00
1:A:175[B]:LEU:HB2	1:A:176[B]:PRO:HD2	1.39	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175[B]:LEU:H	1:B:175[B]:LEU:HD22	1.30	0.92
1:B:175[B]:LEU:HB2	1:B:176[B]:PRO:CD	1.97	0.91
1:B:65:PHE:O	1:B:66:VAL:HB	1.71	0.90
1:B:174[A]:GLU:O	1:B:175[A]:LEU:HG	1.72	0.89
1:A:143:ILE:O	1:A:179[B]:ASP:HB3	1.75	0.87
1:B:286:GLY:HA2	1:B:322:VAL:HG13	1.54	0.86
1:A:232:TRP:CZ3	1:A:267:TRP:O	2.27	0.85
1:A:178[B]:ILE:HA	1:A:179[B]:ASP:HB2	1.58	0.85
1:B:175[B]:LEU:H	1:B:175[B]:LEU:CD2	1.89	0.85
1:B:186:ASN:O	1:B:187:HIS:HB2	1.76	0.85
1:B:119:GLY:HA3	1:B:138:GLU:HB3	1.57	0.84
1:B:118:ALA:CB	1:B:138:GLU:OE1	2.26	0.84
1:B:232:TRP:CZ3	1:B:267:TRP:O	2.29	0.84
1:A:174[A]:GLU:O	1:A:175[A]:LEU:HB2	1.80	0.81
1:A:175[B]:LEU:CB	1:A:176[B]:PRO:CD	2.59	0.80
1:A:67:ASN:HB2	1:A:68:PRO:HD2	1.61	0.80
1:A:289:PRO:O	1:A:290:ALA:HB3	1.82	0.80
1:B:66:VAL:O	1:B:67:ASN:CG	2.24	0.80
1:B:143:ILE:O	1:B:179[B]:ASP:HB3	1.82	0.80
1:A:186:ASN:O	1:A:187:HIS:HB2	1.80	0.79
1:A:66:VAL:O	1:A:67:ASN:CG	2.27	0.78
1:B:178[B]:ILE:HA	1:B:179[B]:ASP:HB2	1.66	0.78
1:A:120:VAL:HG22	1:A:141:GLU:HA	1.65	0.77
1:A:118:ALA:CB	1:A:138:GLU:OE1	2.33	0.76
1:B:175[B]:LEU:CB	1:B:176[B]:PRO:CD	2.60	0.75
1:B:66:VAL:O	1:B:67:ASN:CB	2.35	0.74
1:B:69:TRP:HH2	1:B:213:LEU:HD13	1.52	0.74
1:B:120:VAL:HG22	1:B:141:GLU:HA	1.70	0.72
1:A:174[A]:GLU:O	1:A:175[A]:LEU:CB	2.38	0.72
1:B:289:PRO:O	1:B:290:ALA:HB3	1.89	0.71
1:A:171:THR:HG1	1:A:174[B]:GLU:HG3	1.54	0.70
1:B:179[B]:ASP:O	1:B:180[B]:ALA:HB2	1.91	0.70
1:B:67:ASN:HB2	1:B:68:PRO:HD2	1.71	0.70
1:B:171:THR:HG1	1:B:174[B]:GLU:HG3	1.58	0.69
1:B:167:ARG:NH2	5:B:611:SO4:O3	2.26	0.69
1:A:286:GLY:HA2	1:A:322:VAL:HG13	1.75	0.69
1:A:119:GLY:HA2	1:A:138:GLU:HB3	1.74	0.68
1:A:179[B]:ASP:O	1:A:180[B]:ALA:HB2	1.93	0.68
1:A:160:MET:CE	4:A:505:DXC:H243	2.25	0.67
1:A:160:MET:HE1	4:A:505:DXC:H243	1.76	0.67
1:A:289:PRO:O	1:A:290:ALA:CB	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175[B]:LEU:HD12	1:A:175[B]:LEU:N	2.03	0.67
1:A:66:VAL:O	1:A:67:ASN:CB	2.41	0.66
1:A:178[B]:ILE:CA	1:A:179[B]:ASP:HB2	2.25	0.66
1:B:66:VAL:O	1:B:67:ASN:ND2	2.29	0.65
1:B:174[A]:GLU:O	1:B:175[A]:LEU:CB	2.43	0.65
1:A:288:CYS:C	1:A:289:PRO:O	2.39	0.65
1:B:186:ASN:O	1:B:187:HIS:CB	2.42	0.64
1:B:119:GLY:CA	1:B:138:GLU:HB3	2.26	0.64
1:A:175[B]:LEU:HB3	1:A:176[B]:PRO:HD2	1.79	0.63
1:A:299:GLY:HA2	1:A:300:PRO:C	2.23	0.62
1:A:67:ASN:CB	1:A:68:PRO:HD2	2.27	0.62
1:B:175[B]:LEU:CD2	1:B:175[B]:LEU:N	2.61	0.62
1:A:119:GLY:CA	1:A:138:GLU:HB3	2.29	0.62
1:A:186:ASN:O	1:A:187:HIS:CB	2.47	0.62
1:B:288:CYS:C	1:B:289:PRO:O	2.41	0.62
1:B:218:TRP:CE3	1:B:219:MET:HE2	2.34	0.62
1:A:213:LEU:HA	1:A:229:GLU:HG2	1.82	0.61
1:A:167:ARG:HH21	1:A:167:ARG:HB3	1.65	0.61
1:B:200:ASN:O	1:B:203:PHE:O	2.18	0.61
1:A:66:VAL:O	1:A:66:VAL:HG23	2.01	0.61
1:B:289:PRO:O	1:B:290:ALA:CB	2.46	0.60
1:A:66:VAL:O	1:A:67:ASN:ND2	2.35	0.59
1:B:66:VAL:O	1:B:66:VAL:HG13	2.02	0.59
1:B:178[B]:ILE:CA	1:B:179[B]:ASP:HB2	2.32	0.58
1:B:218:TRP:CE3	1:B:219:MET:CE	2.86	0.58
1:B:167:ARG:HH21	1:B:167:ARG:HB3	1.68	0.58
4:A:504:DXC:H243	1:B:160:MET:HE1	1.84	0.58
1:A:167:ARG:NH2	5:A:508:SO4:O1	2.33	0.58
1:B:299:GLY:HA2	1:B:300:PRO:C	2.28	0.58
1:B:213:LEU:HA	1:B:229:GLU:HG2	1.84	0.57
1:B:67:ASN:CB	1:B:68:PRO:HD2	2.34	0.57
1:B:69:TRP:CH2	1:B:213:LEU:HD13	2.37	0.57
1:B:118:ALA:HB3	6:B:710:HOH:O	2.04	0.57
1:B:174[A]:GLU:O	1:B:175[A]:LEU:CG	2.50	0.57
1:B:120:VAL:O	1:B:121:ARG:HB2	2.05	0.56
1:B:123:ALA:O	1:B:124:GLY:O	2.23	0.56
1:A:67:ASN:HB2	1:A:68:PRO:CD	2.33	0.56
1:B:218:TRP:HE3	1:B:219:MET:HE2	1.70	0.56
1:A:65:PHE:O	1:A:66:VAL:HG22	2.06	0.55
1:A:172:ILE:HG23	1:A:199:LEU:HD13	1.88	0.55
4:A:505:DXC:H13	4:A:505:DXC:H242	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLY:CA	1:A:322:VAL:HG13	2.37	0.54
1:B:179[B]:ASP:O	1:B:180[B]:ALA:CB	2.55	0.54
1:B:66:VAL:O	1:B:67:ASN:HB3	2.07	0.54
1:B:210:PHE:HB3	1:B:270:TRP:CH2	2.42	0.54
1:B:388:ASN:O	1:B:389:ASP:HB2	2.07	0.54
4:A:504:DXC:H242	4:A:504:DXC:H13	1.89	0.53
1:A:210:PHE:HB3	1:A:270:TRP:CH2	2.42	0.53
1:B:120:VAL:CG1	1:B:122:GLU:OE2	2.56	0.53
1:B:179[A]:ASP:HB3	1:B:206:GLU:O	2.08	0.53
1:A:171:THR:OG1	1:A:174[A]:GLU:OE1	2.27	0.53
4:A:504:DXC:H243	1:B:160:MET:CE	2.37	0.53
1:B:66:VAL:O	1:B:66:VAL:CG1	2.56	0.53
1:A:179[B]:ASP:O	1:A:180[B]:ALA:CB	2.57	0.52
1:B:251:SER:HB3	1:B:268:GLY:HA2	1.92	0.52
1:B:227:VAL:O	1:B:228:ILE:HD12	2.08	0.52
1:A:119:GLY:C	1:A:120:VAL:HG23	2.35	0.52
1:A:218:TRP:CE3	1:A:219:MET:HE2	2.45	0.52
1:B:178[B]:ILE:HG22	1:B:180[B]:ALA:H	1.75	0.52
4:A:507:DXC:H182	4:B:607:DXC:H203	1.92	0.51
1:A:120:VAL:HG12	1:A:121:ARG:H	1.74	0.51
1:A:258:THR:HG21	4:A:507:DXC:H3	1.92	0.51
1:A:249:THR:OG1	1:A:269:SER:OG	2.29	0.51
1:A:120:VAL:O	1:A:121:ARG:HB2	2.10	0.50
1:B:357:PRO:HB2	1:B:358:PRO:HD3	1.93	0.50
1:B:64:ARG:HA	1:B:70:PRO:HD3	1.93	0.50
1:B:384:ARG:HD3	6:B:750:HOH:O	2.11	0.50
1:B:120:VAL:HG12	1:B:122:GLU:OE2	2.11	0.50
1:A:64:ARG:HA	1:A:70:PRO:HD3	1.94	0.49
1:B:120:VAL:HG12	1:B:121:ARG:N	2.28	0.49
4:B:601:DXC:H203	4:B:603:DXC:H182	1.94	0.49
1:A:285:THR:HG21	1:A:291:PHE:CZ	2.47	0.49
1:A:125:LEU:C	1:A:125:LEU:HD23	2.38	0.49
1:A:120:VAL:HG12	1:A:121:ARG:N	2.27	0.49
1:A:179[A]:ASP:O	1:A:208:ARG:N	2.27	0.49
1:B:63:GLY:O	1:B:70:PRO:HD2	2.13	0.49
1:B:175[A]:LEU:HB3	1:B:177[A]:PRO:HD3	1.95	0.48
1:B:120:VAL:HG12	1:B:121:ARG:H	1.78	0.48
1:A:175[B]:LEU:H	1:A:175[B]:LEU:CD1	2.03	0.48
1:A:178[B]:ILE:HG22	1:A:180[B]:ALA:H	1.79	0.48
1:A:218:TRP:CE3	1:A:219:MET:CE	2.97	0.47
1:B:273:LEU:HD22	1:B:278:ARG:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:607:DXC:H13	4:B:607:DXC:H242	1.95	0.47
1:A:167:ARG:NH2	1:B:171:THR:HG21	2.29	0.47
1:A:232:TRP:CE3	1:A:250:PRO:HA	2.50	0.47
1:B:66:VAL:C	1:B:67:ASN:CG	2.82	0.47
1:B:174[A]:GLU:N	1:B:174[A]:GLU:OE1	2.48	0.47
1:A:175[B]:LEU:HB2	1:A:176[B]:PRO:CD	2.20	0.47
1:A:216:LEU:HB2	1:A:229:GLU:CD	2.40	0.47
1:B:119:GLY:C	1:B:120:VAL:HG23	2.40	0.47
1:B:171:THR:OG1	1:B:174[A]:GLU:OE1	2.28	0.47
1:B:285:THR:HG21	1:B:291:PHE:CZ	2.50	0.47
4:B:601:DXC:H242	4:B:601:DXC:H13	1.96	0.47
1:A:218:TRP:HE3	1:A:219:MET:HE2	1.79	0.46
1:B:67:ASN:HB2	1:B:68:PRO:CD	2.43	0.46
1:B:340:MET:SD	1:B:378:LEU:HD22	2.55	0.46
1:B:180[A]:ALA:HA	1:B:208:ARG:O	2.14	0.46
1:B:172:ILE:O	1:B:175[B]:LEU:CD2	2.63	0.46
1:B:258:THR:HG21	4:B:603:DXC:H3	1.97	0.46
1:A:120:VAL:CG1	1:A:122:GLU:OE2	2.64	0.46
1:A:110:TYR:OH	1:A:118:ALA:CB	2.64	0.46
1:B:68:PRO:HD3	6:B:758:HOH:O	2.15	0.46
1:A:146:THR:O	1:A:147:ASP:C	2.59	0.45
1:A:156:PRO:HD2	3:A:503:3PE:H362	1.98	0.45
1:A:67:ASN:CB	1:A:68:PRO:CD	2.92	0.45
1:A:120:VAL:HG12	1:A:122:GLU:OE2	2.17	0.45
1:A:111:PHE:CD2	1:A:175[B]:LEU:HA	2.52	0.45
1:B:94:PRO:O	1:B:95:SER:HB2	2.16	0.44
4:A:507:DXC:C8	4:B:602:DXC:H222	2.48	0.44
1:B:111:PHE:CD2	1:B:175[B]:LEU:HA	2.52	0.44
1:A:167:ARG:HH21	1:A:167:ARG:CB	2.31	0.44
1:A:172:ILE:HA	1:A:175[B]:LEU:HD11	1.99	0.44
1:A:227:VAL:O	1:A:228:ILE:HD12	2.18	0.44
1:B:160:MET:HE3	1:B:160:MET:HB3	1.85	0.43
1:A:66:VAL:O	1:A:67:ASN:HB3	2.14	0.43
1:A:180[A]:ALA:HA	1:A:208:ARG:O	2.18	0.43
1:A:253:HIS:CE1	1:A:284:ASP:HB3	2.52	0.43
1:B:185:HIS:HB2	1:B:255:CYS:SG	2.58	0.43
1:B:118:ALA:HA	1:B:121:ARG:NH1	2.32	0.43
1:B:218:TRP:CZ3	1:B:219:MET:CE	3.01	0.43
1:A:66:VAL:C	1:A:67:ASN:CG	2.86	0.43
1:A:357:PRO:HB2	1:A:358:PRO:HD3	2.00	0.43
1:B:69:TRP:H	1:B:69:TRP:CD1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ILE:HG12	1:B:174[A]:GLU:HG2	2.01	0.43
1:A:288:CYS:HG	1:A:290:ALA:HB3	1.84	0.43
1:B:178[A]:ILE:HA	1:B:179[A]:ASP:HA	1.72	0.42
1:B:215:LEU:HD13	1:B:265:VAL:HG11	2.02	0.42
1:A:178[A]:ILE:HA	1:A:179[A]:ASP:HA	1.73	0.42
1:A:112:ILE:HG12	1:A:174[A]:GLU:HG2	2.00	0.42
1:A:280:PHE:O	1:A:304:ALA:HA	2.19	0.42
1:B:125:LEU:HD23	1:B:125:LEU:C	2.45	0.42
1:A:123:ALA:O	1:A:124:GLY:O	2.36	0.42
1:B:174[A]:GLU:O	1:B:175[A]:LEU:HB2	2.19	0.42
1:A:288:CYS:SG	1:A:289:PRO:O	2.77	0.42
1:A:174[A]:GLU:OE1	1:A:174[A]:GLU:N	2.52	0.42
1:B:172:ILE:HD13	1:B:199:LEU:HG	2.02	0.42
1:B:253:HIS:CE1	1:B:284:ASP:HB3	2.55	0.42
1:A:172:ILE:O	1:A:175[B]:LEU:CD1	2.68	0.42
1:B:232:TRP:CE3	1:B:250:PRO:HA	2.55	0.42
1:B:273:LEU:HD22	1:B:278:ARG:CD	2.50	0.42
1:B:342:ILE:C	1:B:343:HIS:O	2.58	0.42
1:B:156:PRO:HD2	3:B:606:3PE:H362	2.00	0.42
1:A:356:GLU:N	1:A:357:PRO:CD	2.83	0.41
1:B:100:LEU:HD23	1:B:100:LEU:HA	1.93	0.41
1:B:232:TRP:CZ3	1:B:266:LEU:HD22	2.55	0.41
1:B:181:VAL:HG23	1:B:207:LEU:HD11	2.02	0.41
1:A:94:PRO:O	1:A:95:SER:HB2	2.20	0.41
1:A:117:GLU:HB2	1:A:121:ARG:NH2	2.36	0.41
1:A:342:ILE:C	1:A:343:HIS:O	2.60	0.41
1:B:218:TRP:HE3	1:B:219:MET:CE	2.30	0.41
1:A:74:ASN:N	1:A:75:PRO:HD2	2.35	0.41
1:A:251:SER:HB3	1:A:268:GLY:HA2	2.01	0.41
1:A:307:PRO:HA	1:A:342:ILE:O	2.20	0.41
1:A:77:ILE:HG22	1:A:78:PRO:HD2	2.02	0.41
1:B:146:THR:O	1:B:147:ASP:C	2.63	0.41
1:A:69:TRP:CD1	1:A:69:TRP:H	2.38	0.41
1:A:249:THR:HG1	1:A:269:SER:HG	1.60	0.41
4:A:507:DXC:H82	4:B:602:DXC:H222	2.01	0.41
1:B:77:ILE:HG22	1:B:78:PRO:HD2	2.02	0.41
1:B:171:THR:OG1	1:B:174[B]:GLU:HG3	2.18	0.41
1:B:191:LEU:HD11	1:B:219:MET:HE1	2.02	0.41
1:B:324:PRO:O	1:B:327:ALA:HB3	2.20	0.41
1:B:65:PHE:O	1:B:66:VAL:CB	2.55	0.41
1:B:175[B]:LEU:HD22	1:B:175[B]:LEU:N	2.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178[B]:ILE:HA	1:A:179[B]:ASP:CB	2.41	0.41
4:B:607:DXC:H201	4:B:607:DXC:H142	1.82	0.41
1:B:110:TYR:OH	1:B:118:ALA:CB	2.69	0.40
1:B:167:ARG:NH1	5:B:611:SO4:O3	2.54	0.40
1:A:273:LEU:HD12	1:A:278:ARG:HD2	2.03	0.40
1:B:177[A]:PRO:HD2	1:B:203:PHE:CZ	2.56	0.40
1:B:343:HIS:O	1:B:344:TRP:CD1	2.75	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	325/393 (83%)	284 (87%)	22 (7%)	19 (6%)	1	1
1	B	325/393 (83%)	281 (86%)	26 (8%)	18 (6%)	1	2
All	All	650/786 (83%)	565 (87%)	48 (7%)	37 (6%)	1	1

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	67	ASN
1	A	119	GLY
1	A	120	VAL
1	A	121	ARG
1	A	187	HIS
1	B	66	VAL
1	B	67	ASN
1	B	119	GLY
1	B	120	VAL
1	B	121	ARG

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Mol	Chain	Res	Type
1	B	187	HIS
1	A	117	GLU
1	A	124	GLY
1	A	179[A]	ASP
1	A	179[B]	ASP
1	A	344	TRP
1	B	117	GLU
1	B	124	GLY
1	B	179[A]	ASP
1	B	179[B]	ASP
1	B	180[A]	ALA
1	B	180[B]	ALA
1	B	290	ALA
1	B	344	TRP
1	A	70	PRO
1	A	180[A]	ALA
1	A	180[B]	ALA
1	A	290	ALA
1	B	70	PRO
1	A	289	PRO
1	B	96	SER
1	A	68	PRO
1	A	96	SER
1	B	289	PRO
1	B	74	ASN
1	A	74	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/352 (83%)	246 (84%)	45 (16%)	2	3
1	B	291/352 (83%)	254 (87%)	37 (13%)	4	6
All	All	582/704 (83%)	500 (86%)	82 (14%)	3	5

All (82) 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	66	VAL
1	A	68	PRO
1	A	71	THR
1	A	72	TRP
1	A	73	LYS
1	A	74	ASN
1	A	96	SER
1	A	100	LEU
1	A	117	GLU
1	A	127	VAL
1	A	130	LEU
1	A	135	VAL
1	A	152	SER
1	A	160	MET
1	A	167	ARG
1	A	175[A]	LEU
1	A	175[B]	LEU
1	A	178[A]	ILE
1	A	178[B]	ILE
1	A	181	VAL
1	A	199	LEU
1	A	213	LEU
1	A	215	LEU
1	A	216	LEU
1	A	228	ILE
1	A	242	ASP
1	A	243	LYS
1	A	251	SER
1	A	265	VAL
1	A	273	LEU
1	A	324	PRO
1	A	329	ARG
1	A	334	VAL
1	A	343	HIS
1	A	344	TRP
1	A	361	LEU
1	A	365	LEU
1	A	366	GLU
1	A	377	VAL
1	A	384	ARG

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Mol	Chain	Res	Type
1	A	386	LEU
1	A	387	ASN
1	B	58	LYS
1	B	59	LYS
1	B	61	LYS
1	B	66	VAL
1	B	68	PRO
1	B	71	THR
1	B	72	TRP
1	B	73	LYS
1	B	74	ASN
1	B	77	ILE
1	B	96	SER
1	B	107	LEU
1	B	117	GLU
1	B	127	VAL
1	B	135	VAL
1	B	160	MET
1	B	167	ARG
1	B	178[A]	ILE
1	B	178[B]	ILE
1	B	213	LEU
1	B	228	ILE
1	B	243	LYS
1	B	251	SER
1	B	324	PRO
1	B	328	VAL
1	B	329	ARG
1	B	334	VAL
1	B	343	HIS
1	B	344	TRP
1	B	349	LEU
1	B	355	LEU
1	B	366	GLU
1	B	367	ARG
1	B	377	VAL
1	B	378	LEU
1	B	384	ARG
1	B	387	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	DXC	A	504	-	31,31,31	0.95	2 (6%)	49,49,49	1.34	7 (14%)
5	SO4	B	611	-	4,4,4	0.67	0	6,6,6	0.63	0
4	DXC	B	610	-	31,31,31	1.03	2 (6%)	49,49,49	2.40	16 (32%)
4	DXC	B	601	-	31,31,31	0.98	1 (3%)	49,49,49	1.38	8 (16%)
4	DXC	B	609	-	31,31,31	1.18	3 (9%)	49,49,49	2.14	13 (26%)
4	DXC	B	603	-	31,31,31	1.32	3 (9%)	49,49,49	3.88	23 (46%)
5	SO4	A	508	-	4,4,4	0.53	0	6,6,6	0.42	0
4	DXC	A	506	-	31,31,31	0.97	1 (3%)	49,49,49	1.34	6 (12%)
4	DXC	B	607	-	31,31,31	1.12	4 (12%)	49,49,49	1.54	12 (24%)
3	3PE	A	503	2	43,43,50	0.97	3 (6%)	46,48,55	1.37	4 (8%)
4	DXC	B	602	-	31,31,31	0.96	1 (3%)	49,49,49	1.22	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DXC	A	505	-	31,31,31	1.00	1 (3%)	49,49,49	1.32	7 (14%)
4	DXC	B	608	-	31,31,31	1.15	3 (9%)	49,49,49	1.61	13 (26%)
4	DXC	A	507	-	31,31,31	1.26	3 (9%)	49,49,49	3.55	20 (40%)
5	SO4	A	509	-	4,4,4	0.49	0	6,6,6	0.30	0
3	3PE	B	606	2	43,43,50	1.04	2 (4%)	46,48,55	1.42	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DXC	A	504	-	-	2/9/71/71	0/4/4/4
4	DXC	B	610	-	-	9/9/71/71	0/4/4/4
4	DXC	B	601	-	-	0/9/71/71	0/4/4/4
4	DXC	B	609	-	-	1/9/71/71	0/4/4/4
4	DXC	B	603	-	-	3/9/71/71	0/4/4/4
4	DXC	A	506	-	-	3/9/71/71	0/4/4/4
4	DXC	B	607	-	-	0/9/71/71	0/4/4/4
3	3PE	A	503	2	-	17/47/47/54	-
4	DXC	B	602	-	-	2/9/71/71	0/4/4/4
4	DXC	A	505	-	-	2/9/71/71	0/4/4/4
4	DXC	B	608	-	-	3/9/71/71	0/4/4/4
4	DXC	A	507	-	-	4/9/71/71	0/4/4/4
3	3PE	B	606	2	-	17/47/47/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	DXC	C12-C11	-4.89	1.47	1.55
3	B	606	3PE	O21-C21	4.82	1.47	1.34
3	A	503	3PE	O21-C21	4.27	1.46	1.34
4	A	507	DXC	C12-C11	-3.16	1.50	1.55
4	A	507	DXC	C12-C17	-3.08	1.50	1.55
4	B	609	DXC	C12-C11	-2.87	1.50	1.55
3	B	606	3PE	O31-C31	2.85	1.41	1.33
4	B	608	DXC	C12-C11	-2.75	1.50	1.55
4	B	608	DXC	C12-C17	-2.57	1.51	1.55
4	A	506	DXC	C12-C11	-2.54	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	607	DXC	C4-C3	-2.53	1.51	1.55
4	B	610	DXC	C4-C3	-2.46	1.51	1.55
4	A	504	DXC	C14-C13	2.39	1.57	1.53
4	A	505	DXC	C12-C11	-2.37	1.51	1.55
4	B	602	DXC	C12-C11	-2.36	1.51	1.55
3	A	503	3PE	O31-C31	2.32	1.40	1.33
4	B	609	DXC	C12-C17	-2.32	1.51	1.55
4	B	607	DXC	C12-C13	-2.31	1.51	1.54
4	A	504	DXC	C12-C11	-2.30	1.51	1.55
4	B	610	DXC	C4-C10	-2.27	1.52	1.56
4	A	507	DXC	C4-C3	-2.26	1.51	1.55
4	B	607	DXC	C20-C12	-2.24	1.50	1.54
4	B	607	DXC	C2-C3	-2.16	1.50	1.53
4	B	603	DXC	C4-C3	-2.13	1.52	1.55
4	B	601	DXC	C20-C12	-2.12	1.50	1.54
4	B	603	DXC	C4-C10	-2.12	1.52	1.56
4	B	609	DXC	C12-C13	-2.12	1.51	1.54
3	A	503	3PE	O31-C3	-2.05	1.40	1.45
4	B	608	DXC	C12-C13	-2.01	1.51	1.54

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	DXC	C12-C11-C9	-14.85	98.73	114.69
4	A	507	DXC	C12-C11-C9	-13.78	99.87	114.69
4	B	603	DXC	C11-C9-C10	-11.63	93.89	109.09
4	A	507	DXC	C11-C9-C10	-11.08	94.61	109.09
4	B	603	DXC	C11-C12-C13	7.85	114.59	107.42
4	B	603	DXC	C8-C9-C10	7.69	119.73	110.52
4	A	507	DXC	C8-C9-C10	6.78	118.64	110.52
4	B	603	DXC	C15-C11-C12	6.71	110.04	103.54
4	A	507	DXC	C12-C17-C19	-6.33	111.81	119.48
4	B	610	DXC	C10-C14-C13	-6.24	106.13	114.29
4	B	609	DXC	C14-C13-C12	6.13	117.50	111.26
4	B	610	DXC	C12-C11-C9	-5.95	108.29	114.69
3	A	503	3PE	O21-C21-C22	5.86	124.15	111.48
4	A	507	DXC	C15-C11-C12	5.66	109.03	103.54
4	B	610	DXC	C4-C10-C9	5.53	118.04	112.43
4	B	603	DXC	C12-C17-C19	-5.15	113.24	119.48
3	B	606	3PE	O21-C21-C22	5.08	122.46	111.48
4	B	603	DXC	C20-C12-C17	-5.05	103.29	111.20
4	B	609	DXC	C10-C14-C13	4.63	120.35	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	609	DXC	C11-C12-C13	4.45	111.48	107.42
4	B	610	DXC	C11-C9-C10	-4.35	103.40	109.09
4	B	609	DXC	C2-C3-C7	-4.34	104.23	111.73
4	B	610	DXC	C12-C17-C19	-4.28	114.30	119.48
4	B	610	DXC	C20-C12-C13	-4.27	104.78	109.06
4	A	507	DXC	C3-C2-C1	-4.24	106.31	112.71
4	A	507	DXC	C14-C10-C4	4.20	117.96	113.70
4	B	610	DXC	C14-C13-C12	-4.18	107.01	111.26
4	B	610	DXC	C2-C3-C4	-3.97	108.44	112.66
4	A	507	DXC	C11-C12-C13	3.94	111.02	107.42
4	B	603	DXC	C3-C2-C1	-3.83	106.93	112.71
4	B	609	DXC	O1-C13-C12	-3.79	104.62	111.02
4	B	603	DXC	C14-C10-C4	3.79	117.55	113.70
4	B	609	DXC	C8-C9-C10	-3.77	106.00	110.52
3	B	606	3PE	O31-C31-O32	-3.72	114.33	123.63
4	B	601	DXC	C2-C3-C7	-3.65	105.42	111.73
4	A	504	DXC	C3-C2-C1	-3.55	107.36	112.71
4	A	505	DXC	C5-C6-C1	-3.54	105.79	110.48
4	B	608	DXC	C21-C19-C17	-3.53	103.01	110.33
4	B	603	DXC	C18-C4-C5	3.50	113.87	108.31
4	A	507	DXC	C18-C4-C5	3.48	113.83	108.31
3	A	503	3PE	O31-C31-O32	-3.46	114.98	123.63
4	A	507	DXC	C7-C3-C4	-3.42	106.57	112.31
4	B	609	DXC	C18-C4-C10	-3.42	106.58	111.18
4	B	610	DXC	C10-C4-C3	3.39	113.22	108.51
4	B	603	DXC	C5-C6-C1	3.39	114.97	110.48
4	B	603	DXC	C7-C3-C4	-3.37	106.65	112.31
4	A	507	DXC	C14-C13-C12	3.34	114.66	111.26
4	B	607	DXC	C18-C4-C10	-3.32	106.72	111.18
4	B	610	DXC	C11-C12-C13	3.28	110.41	107.42
4	A	504	DXC	C5-C4-C10	3.23	116.35	111.34
4	B	603	DXC	C8-C7-C3	-3.16	105.73	111.84
4	B	609	DXC	C6-C5-C4	-3.15	107.43	112.74
4	B	607	DXC	C5-C4-C10	3.12	116.18	111.34
4	A	506	DXC	C21-C19-C17	-3.11	103.87	110.33
4	B	603	DXC	C8-C9-C11	3.07	117.17	112.08
4	A	505	DXC	C3-C2-C1	-3.06	108.09	112.71
4	B	607	DXC	C6-C5-C4	3.05	117.89	112.74
4	B	610	DXC	C5-C4-C10	-3.03	106.63	111.34
4	B	608	DXC	C18-C4-C3	-3.02	105.39	110.44
4	A	505	DXC	C5-C4-C10	3.02	116.03	111.34
4	B	603	DXC	C2-C1-C6	-3.02	106.94	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	608	DXC	C12-C11-C9	-2.99	111.48	114.69
4	B	608	DXC	C24-C19-C21	2.97	114.94	110.34
4	B	603	DXC	C14-C10-C9	-2.95	106.12	110.81
4	B	609	DXC	C10-C4-C3	2.91	112.56	108.51
3	B	606	3PE	O22-C21-C22	-2.89	112.48	123.78
4	B	607	DXC	C14-C13-C12	-2.88	108.33	111.26
4	A	507	DXC	C14-C10-C9	-2.86	106.27	110.81
4	A	507	DXC	C20-C12-C17	-2.85	106.73	111.20
4	B	608	DXC	C14-C10-C4	-2.85	110.81	113.70
4	B	601	DXC	C10-C14-C13	-2.85	110.57	114.29
4	B	608	DXC	C21-C22-C23	-2.84	104.91	112.49
4	A	507	DXC	C8-C7-C3	-2.81	106.39	111.84
4	B	603	DXC	C24-C19-C17	-2.80	108.68	112.88
4	B	607	DXC	C10-C14-C13	-2.79	110.64	114.29
4	A	505	DXC	C24-C19-C17	-2.76	108.74	112.88
4	A	506	DXC	C17-C12-C11	-2.73	97.37	100.11
4	B	607	DXC	C2-C3-C7	-2.71	107.05	111.73
4	B	609	DXC	C17-C12-C13	-2.68	115.25	117.67
4	B	608	DXC	C10-C4-C3	2.67	112.22	108.51
3	A	503	3PE	O22-C21-C22	-2.65	113.40	123.78
4	B	610	DXC	C3-C2-C1	-2.65	108.71	112.71
4	A	504	DXC	C18-C4-C5	-2.65	104.09	108.31
4	A	507	DXC	C8-C9-C11	2.62	116.44	112.08
4	B	603	DXC	O2-C1-C2	2.59	115.01	109.84
4	B	601	DXC	C5-C6-C1	2.59	113.91	110.48
4	A	507	DXC	C2-C1-C6	-2.58	107.47	110.62
4	B	609	DXC	C2-C3-C4	2.57	115.40	112.66
4	B	608	DXC	C12-C17-C19	-2.56	116.39	119.48
4	A	507	DXC	C5-C6-C1	2.55	113.86	110.48
4	A	507	DXC	C6-C5-C4	-2.55	108.43	112.74
4	B	603	DXC	C22-C21-C19	-2.55	109.69	114.46
4	B	607	DXC	O2-C1-C2	-2.54	104.79	109.84
4	B	602	DXC	C10-C4-C3	2.54	112.04	108.51
3	B	606	3PE	C2-O21-C21	2.51	123.81	117.80
4	A	505	DXC	C18-C4-C5	-2.48	104.36	108.31
4	A	504	DXC	O1-C13-C14	2.47	114.15	109.12
4	A	507	DXC	C24-C19-C17	-2.45	109.21	112.88
4	A	506	DXC	C12-C11-C9	2.42	117.30	114.69
4	A	506	DXC	C24-C19-C21	2.39	114.04	110.34
4	A	504	DXC	C5-C6-C1	-2.39	107.32	110.48
4	B	602	DXC	C21-C19-C17	-2.35	105.46	110.33
4	B	609	DXC	C4-C10-C9	-2.29	110.10	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	610	DXC	C18-C4-C10	-2.29	108.10	111.18
4	B	610	DXC	C17-C12-C13	2.29	119.72	117.67
4	B	603	DXC	C18-C4-C3	-2.27	106.64	110.44
4	B	608	DXC	C22-C21-C19	2.27	118.70	114.46
4	B	608	DXC	C20-C12-C17	-2.27	107.65	111.20
4	A	505	DXC	C24-C19-C21	-2.26	106.84	110.34
4	A	504	DXC	C12-C17-C19	-2.25	116.76	119.48
3	A	503	3PE	O31-C3-C2	-2.25	101.92	108.40
4	B	610	DXC	C17-C12-C11	2.24	102.36	100.11
4	B	603	DXC	C6-C5-C4	-2.24	108.96	112.74
4	B	610	DXC	C7-C8-C9	-2.23	108.60	112.16
4	A	507	DXC	C18-C4-C3	-2.22	106.73	110.44
4	A	506	DXC	C8-C9-C10	2.22	113.17	110.52
4	B	602	DXC	C16-C17-C19	-2.21	108.83	112.18
4	A	504	DXC	C4-C10-C9	-2.18	110.22	112.43
4	B	602	DXC	C17-C12-C11	-2.17	97.94	100.11
4	B	607	DXC	O4-C23-C22	2.17	120.86	114.00
3	B	606	3PE	O31-C3-C2	-2.16	102.16	108.40
4	B	601	DXC	C18-C4-C10	-2.16	108.28	111.18
4	B	601	DXC	C7-C8-C9	-2.15	108.74	112.16
4	B	601	DXC	C14-C13-C12	-2.14	109.08	111.26
4	B	601	DXC	C5-C4-C10	2.14	114.66	111.34
4	B	607	DXC	C10-C4-C3	2.11	111.45	108.51
4	B	603	DXC	C2-C3-C4	-2.11	110.42	112.66
4	B	607	DXC	C21-C22-C23	-2.10	106.89	112.49
4	B	602	DXC	C24-C19-C21	2.08	113.56	110.34
4	B	608	DXC	C2-C3-C7	-2.08	108.14	111.73
4	B	602	DXC	C11-C9-C10	-2.07	106.38	109.09
3	B	606	3PE	O31-C31-C32	2.07	118.14	111.83
4	A	506	DXC	C17-C12-C13	2.06	119.52	117.67
4	B	603	DXC	O4-C23-C22	2.05	120.49	114.00
4	B	607	DXC	C7-C8-C9	-2.05	108.89	112.16
4	B	608	DXC	C7-C8-C9	-2.05	108.89	112.16
4	B	609	DXC	C16-C17-C12	-2.05	101.55	103.54
4	A	505	DXC	C4-C10-C9	-2.04	110.36	112.43
4	B	607	DXC	C2-C1-C6	-2.03	108.14	110.62
4	B	601	DXC	O4-C23-C22	2.03	120.41	114.00
4	B	608	DXC	O4-C23-C22	2.03	120.40	114.00

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	3PE	C1-O11-P-O12
3	A	503	3PE	C1-O11-P-O13
3	B	606	3PE	C1-O11-P-O12
3	B	606	3PE	C1-O11-P-O13
4	B	610	DXC	C12-C17-C19-C24
4	B	610	DXC	C16-C17-C19-C21
3	A	503	3PE	O32-C31-O31-C3
3	A	503	3PE	C32-C31-O31-C3
3	B	606	3PE	C32-C31-O31-C3
4	B	610	DXC	C24-C19-C21-C22
3	B	606	3PE	O32-C31-O31-C3
4	B	610	DXC	C16-C17-C19-C24
4	B	608	DXC	C24-C19-C21-C22
4	B	610	DXC	C12-C17-C19-C21
3	A	503	3PE	C31-C32-C33-C34
4	A	507	DXC	C17-C19-C21-C22
4	B	603	DXC	C17-C19-C21-C22
3	B	606	3PE	C31-C32-C33-C34
4	A	507	DXC	C24-C19-C21-C22
4	A	507	DXC	C19-C21-C22-C23
4	B	603	DXC	C19-C21-C22-C23
3	A	503	3PE	C21-C22-C23-C24
4	B	603	DXC	C24-C19-C21-C22
3	B	606	3PE	C21-C22-C23-C24
3	B	606	3PE	C34-C35-C36-C37
3	A	503	3PE	C34-C35-C36-C37
4	B	610	DXC	C17-C19-C21-C22
3	A	503	3PE	C3A-C3B-C3C-C3D
4	B	602	DXC	C24-C19-C21-C22
4	B	609	DXC	C16-C17-C19-C21
3	B	606	3PE	O11-C1-C2-C3
3	B	606	3PE	C3A-C3B-C3C-C3D
4	A	506	DXC	C24-C19-C21-C22
3	B	606	3PE	C37-C38-C39-C3A
3	A	503	3PE	C37-C38-C39-C3A
3	B	606	3PE	O11-C1-C2-O21
3	A	503	3PE	C1-O11-P-O14
3	A	503	3PE	O11-C1-C2-C3
3	A	503	3PE	O11-C1-C2-O21
3	A	503	3PE	C29-C2A-C2B-C2C
3	B	606	3PE	C24-C25-C26-C27
3	A	503	3PE	C23-C24-C25-C26
3	B	606	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
3	B	606	3PE	C29-C2A-C2B-C2C
4	B	608	DXC	C21-C22-C23-O4
3	A	503	3PE	C24-C25-C26-C27
4	B	608	DXC	C21-C22-C23-O3
4	B	610	DXC	C19-C21-C22-C23
4	B	610	DXC	C21-C22-C23-O4
3	B	606	3PE	O31-C31-C32-C33
4	A	505	DXC	C21-C22-C23-O4
3	A	503	3PE	O31-C31-C32-C33
3	B	606	3PE	C33-C34-C35-C36
4	A	506	DXC	C21-C22-C23-O3
4	A	506	DXC	C21-C22-C23-O4
4	B	610	DXC	C21-C22-C23-O3
4	A	505	DXC	C21-C22-C23-O3
4	B	602	DXC	C21-C22-C23-O3
3	B	606	3PE	O32-C31-C32-C33
4	A	504	DXC	C21-C22-C23-O4
3	A	503	3PE	O32-C31-C32-C33
4	A	504	DXC	C21-C22-C23-O3
4	A	507	DXC	C12-C17-C19-C24

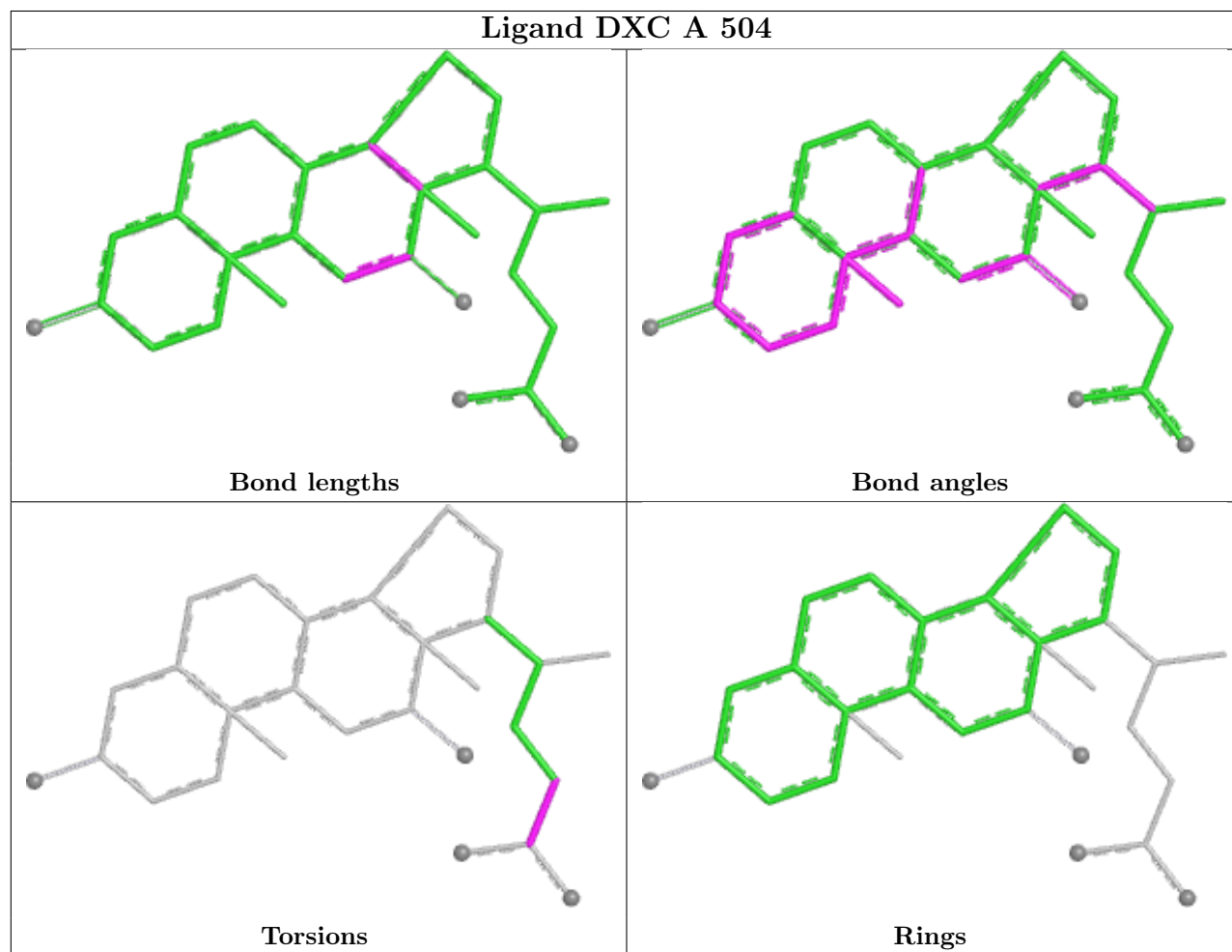
There are no ring outliers.

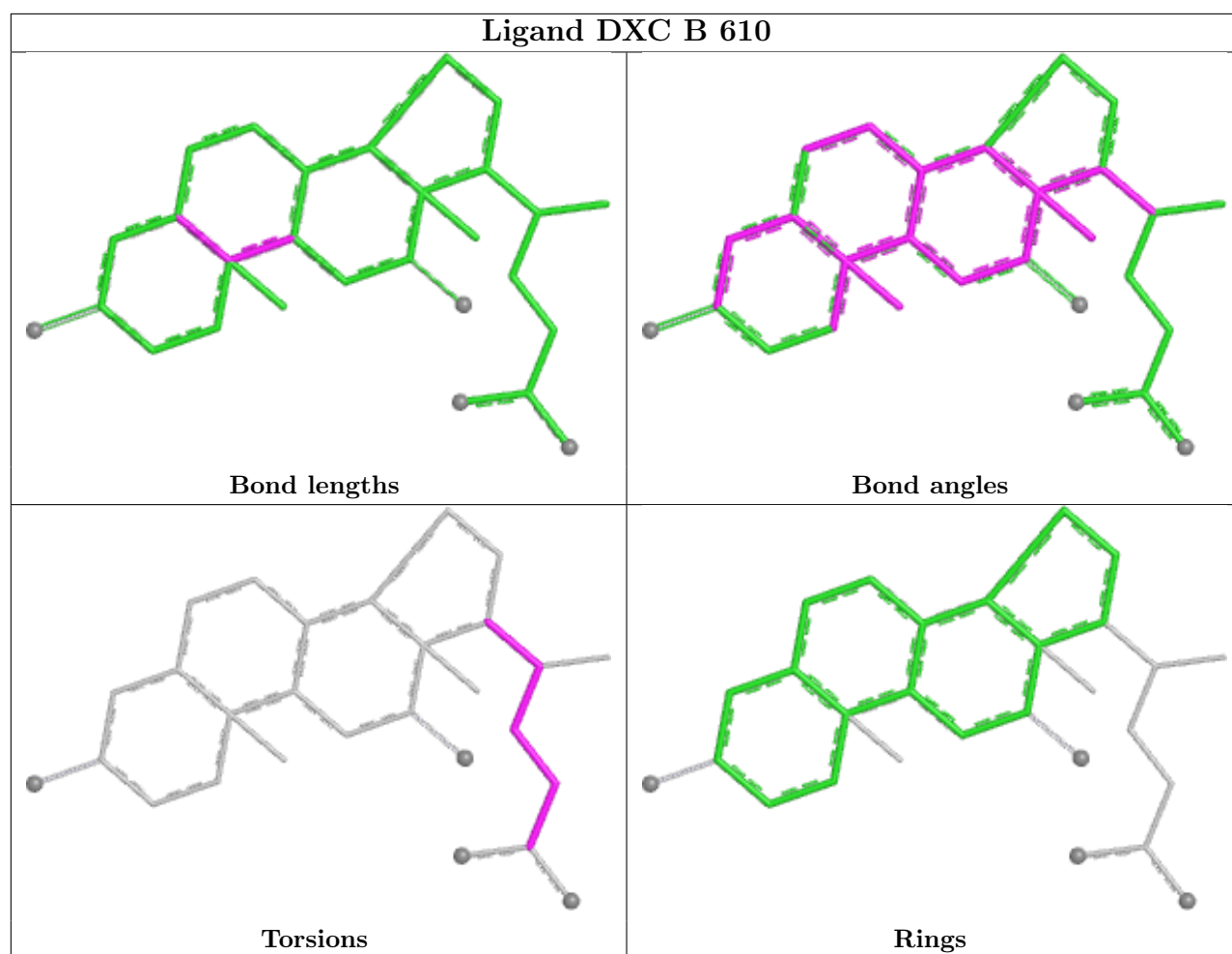
11 monomers are involved in 20 short contacts:

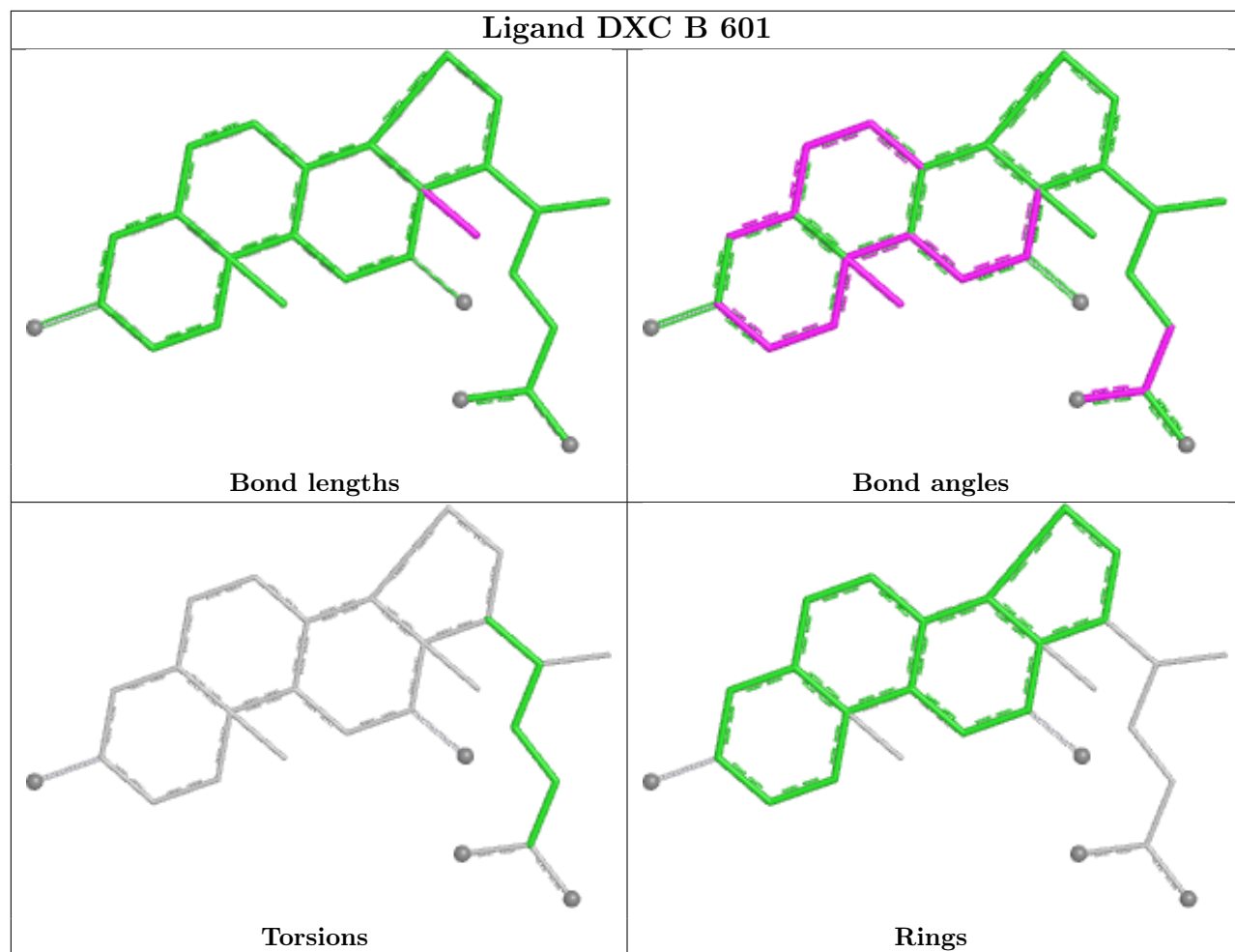
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	DXC	3	0
5	B	611	SO4	2	0
4	B	601	DXC	2	0
4	B	603	DXC	2	0
5	A	508	SO4	1	0
4	B	607	DXC	3	0
3	A	503	3PE	1	0
4	B	602	DXC	2	0
4	A	505	DXC	3	0
4	A	507	DXC	4	0
3	B	606	3PE	1	0

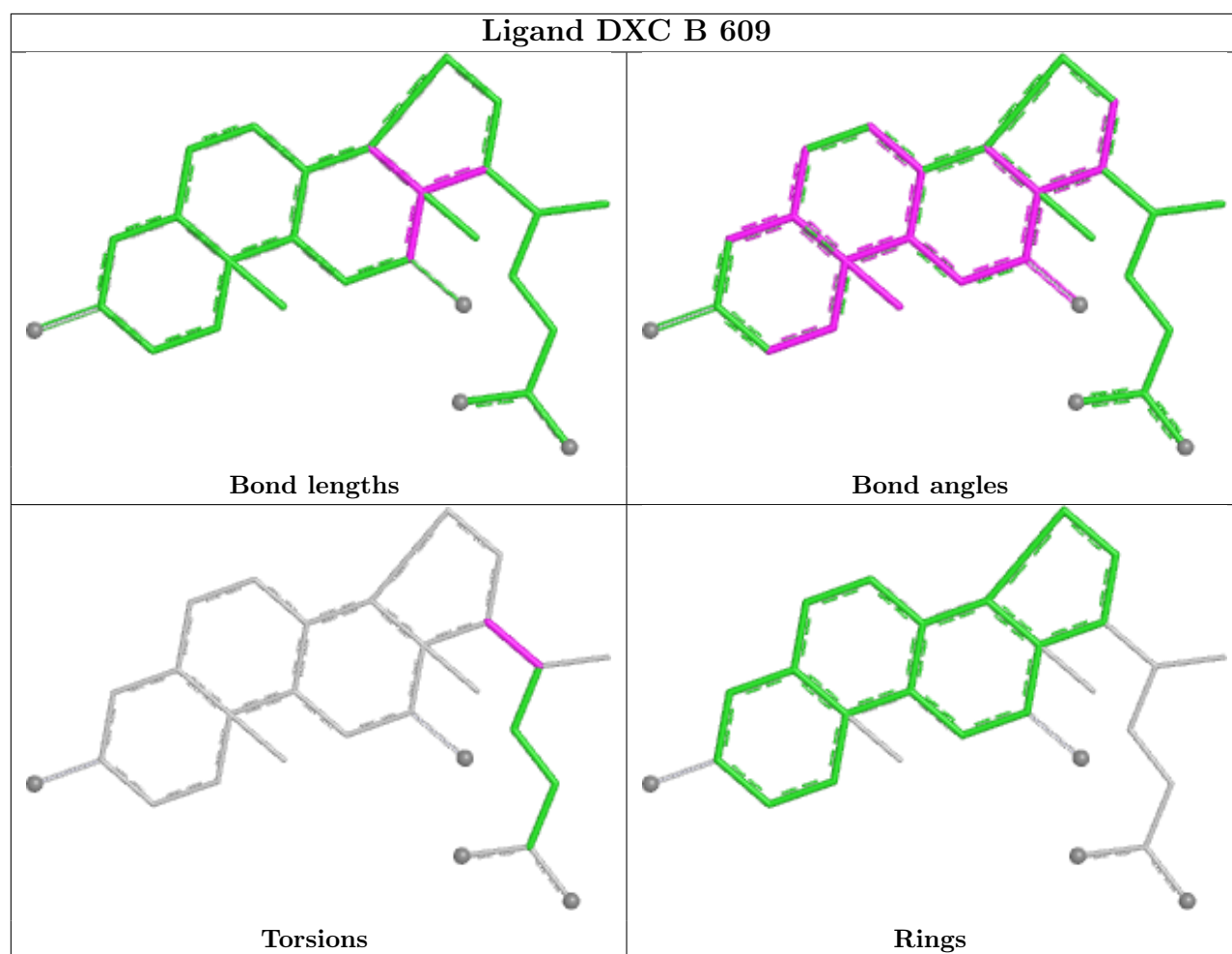
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

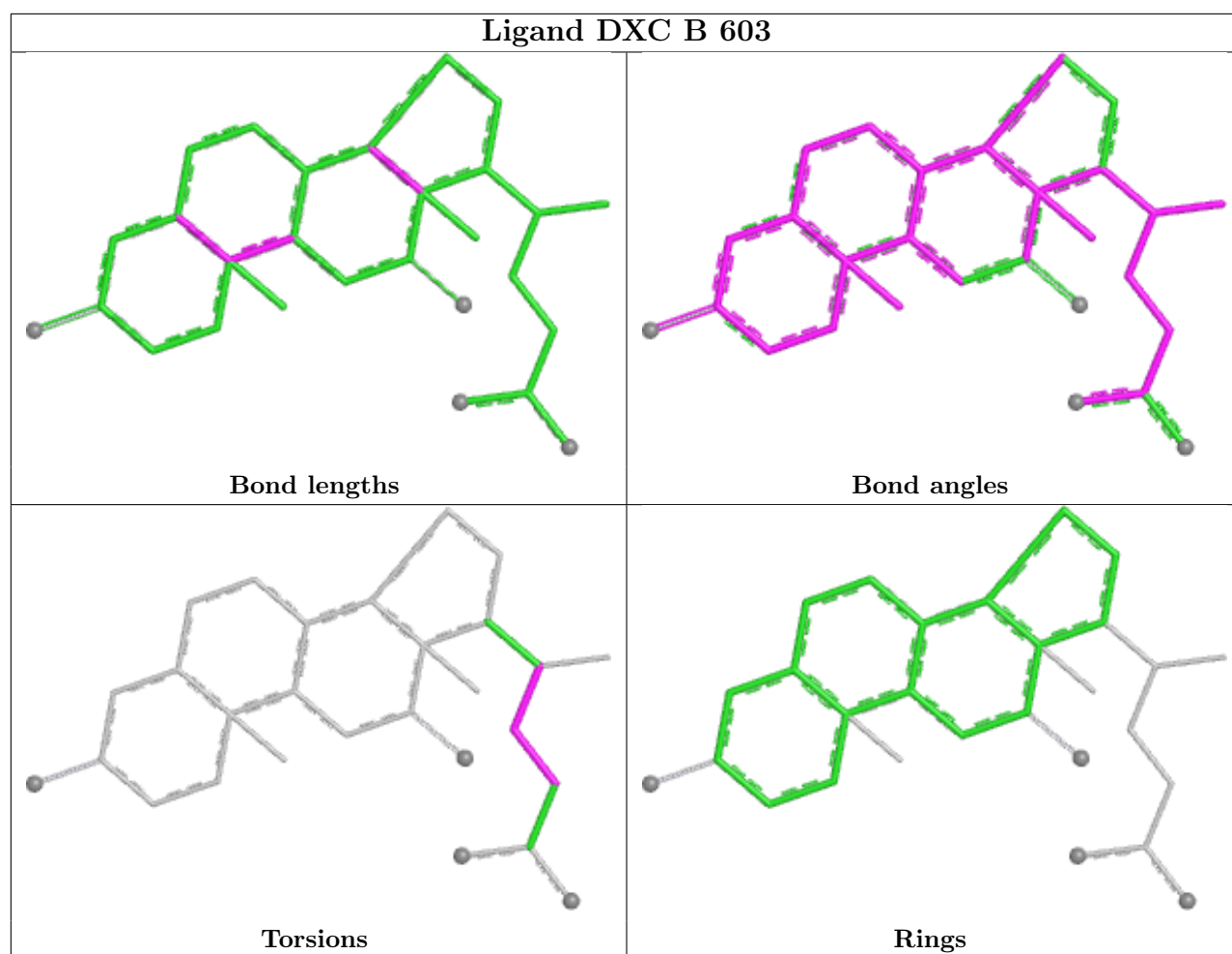
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

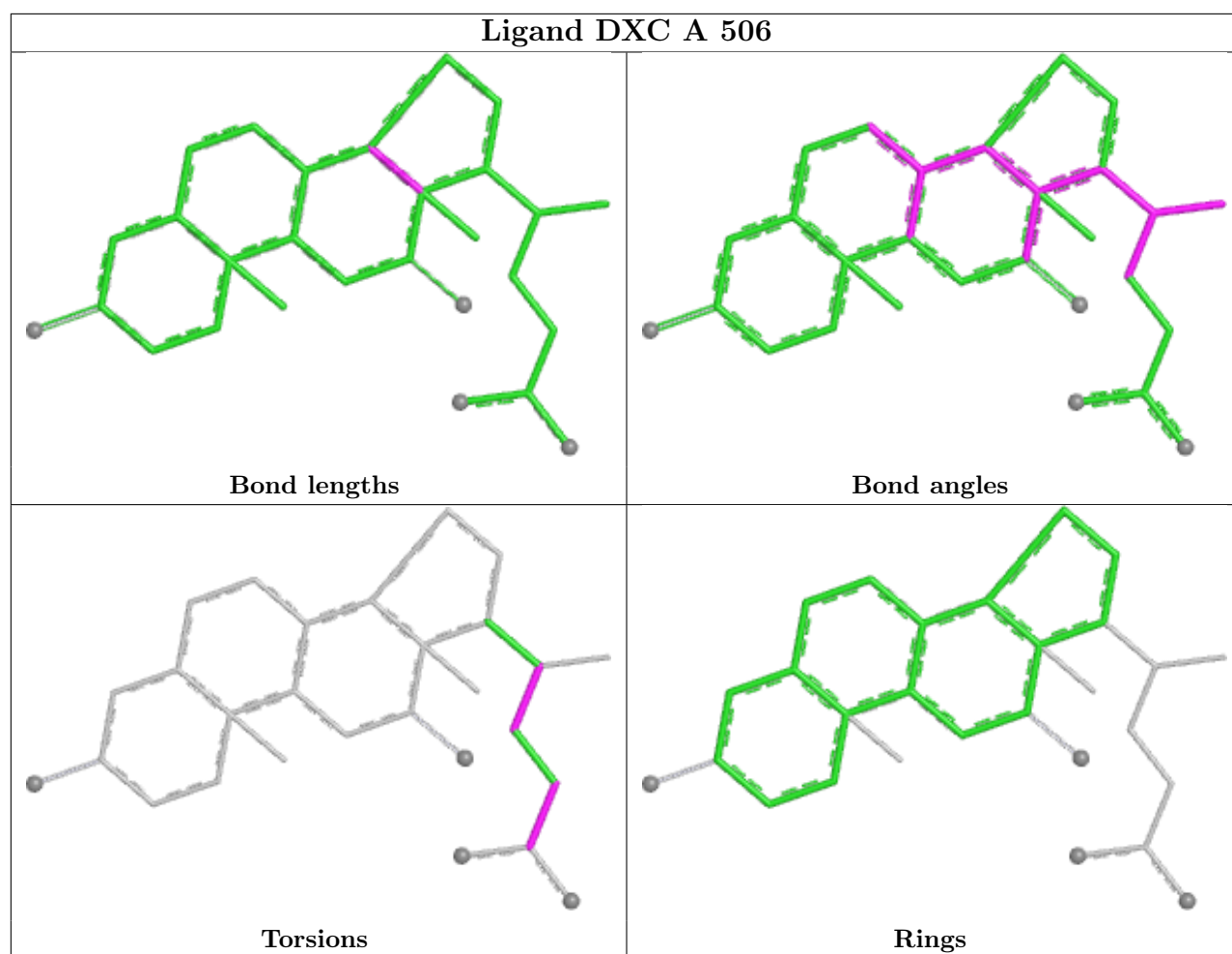




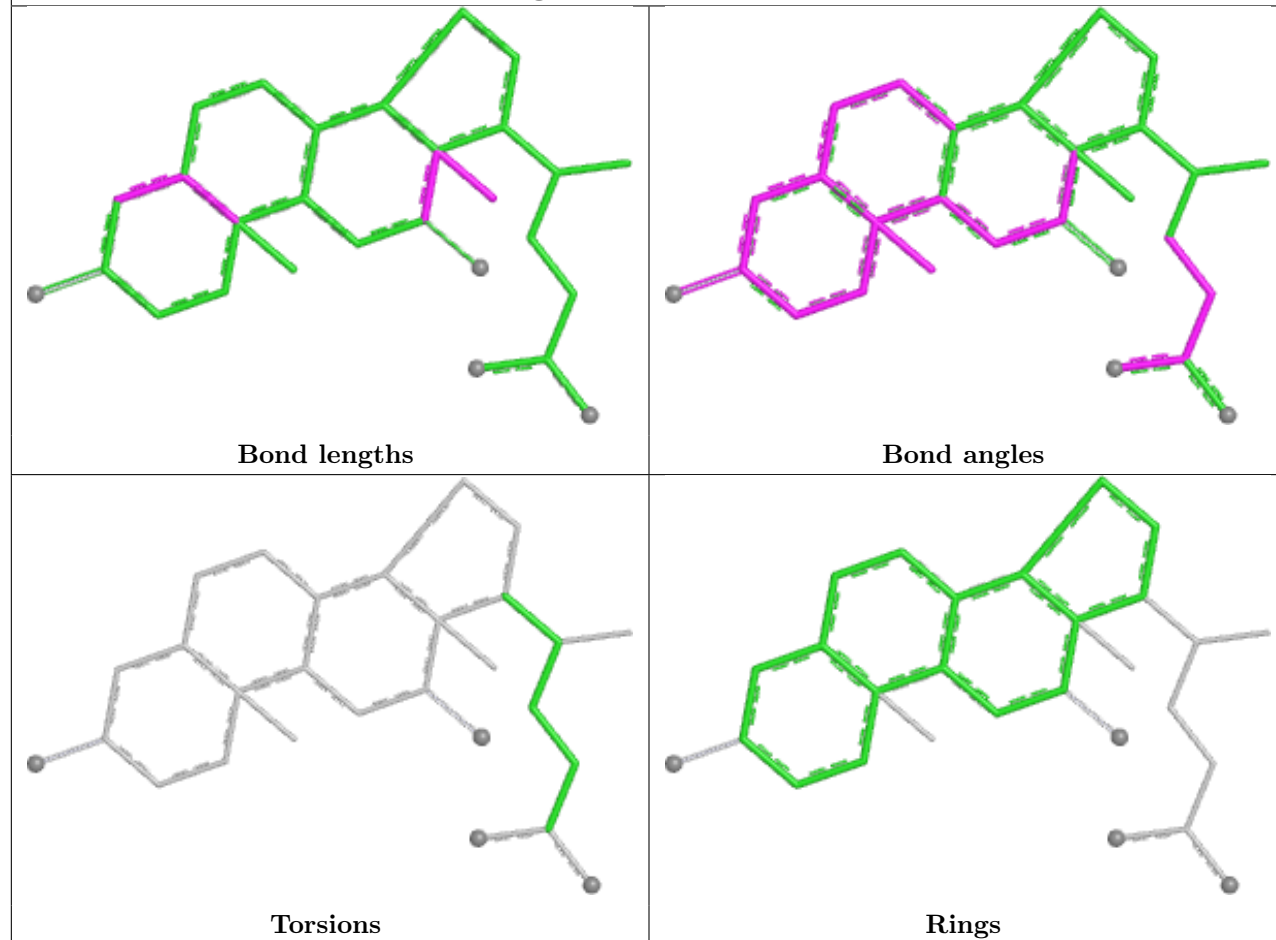




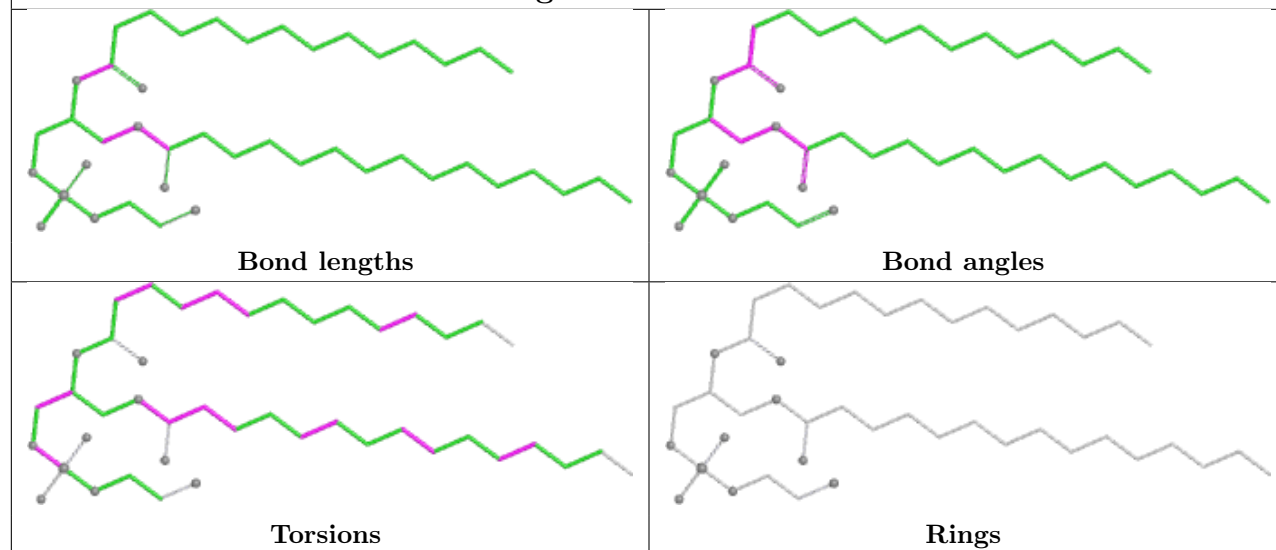


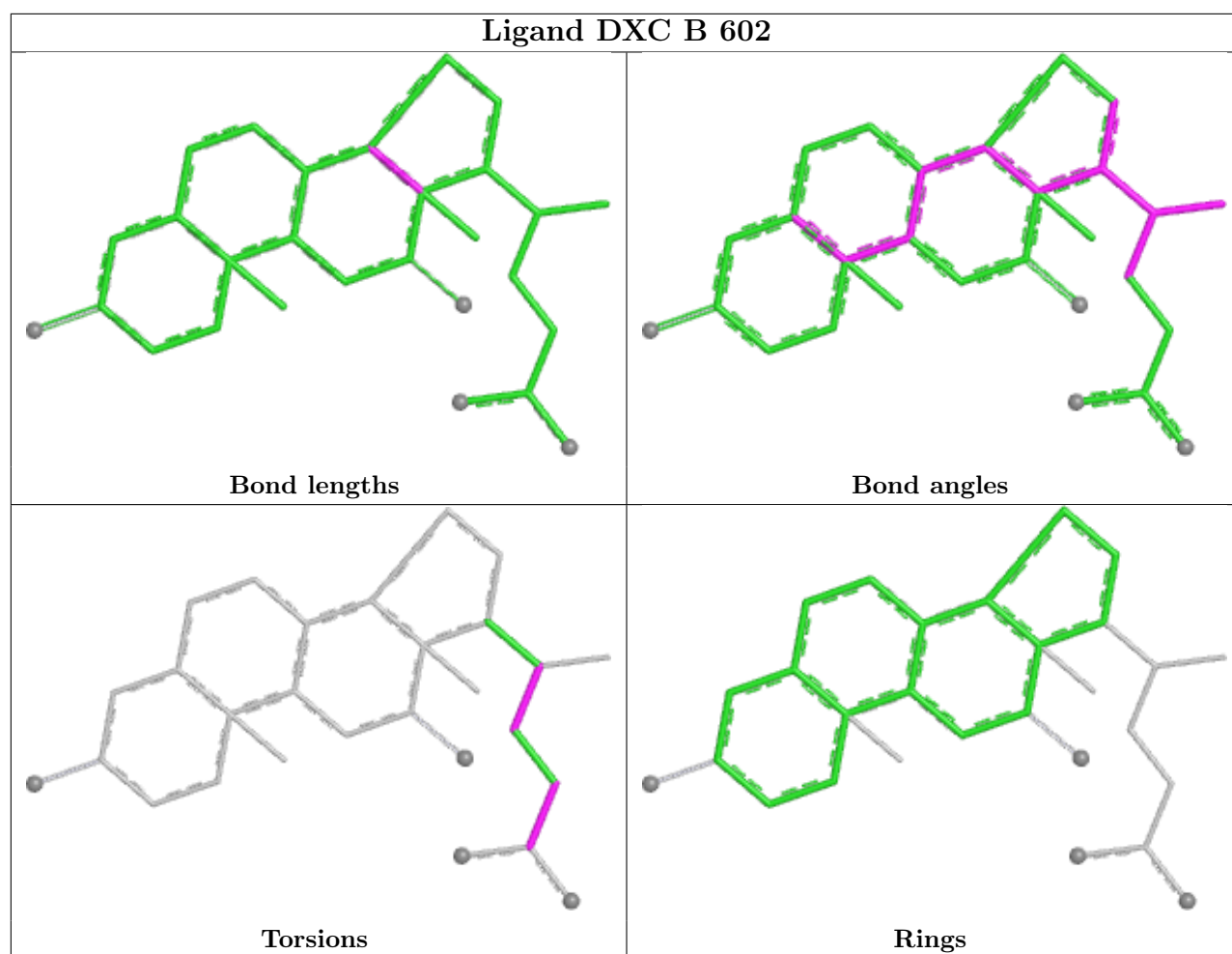


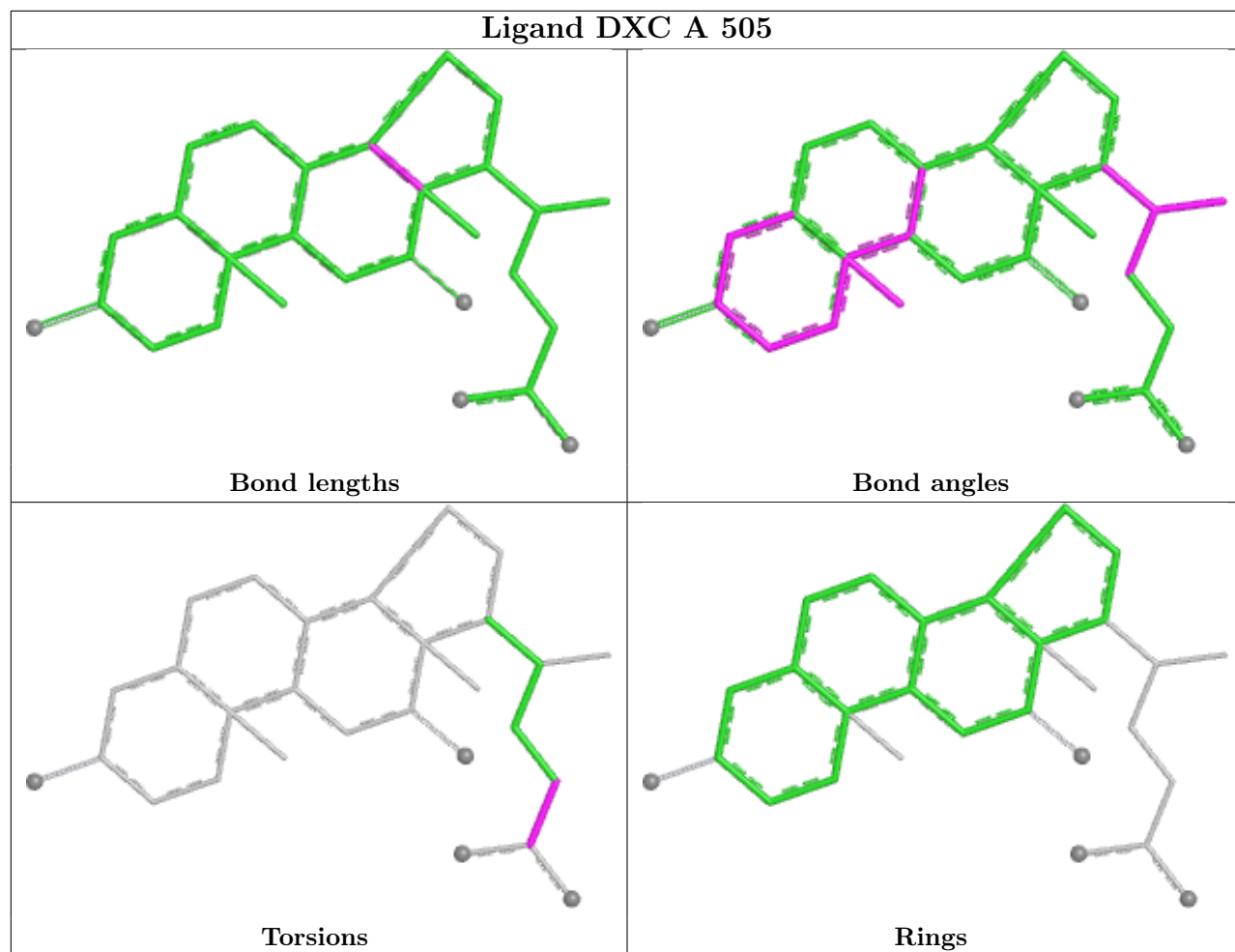
Ligand DXC B 607

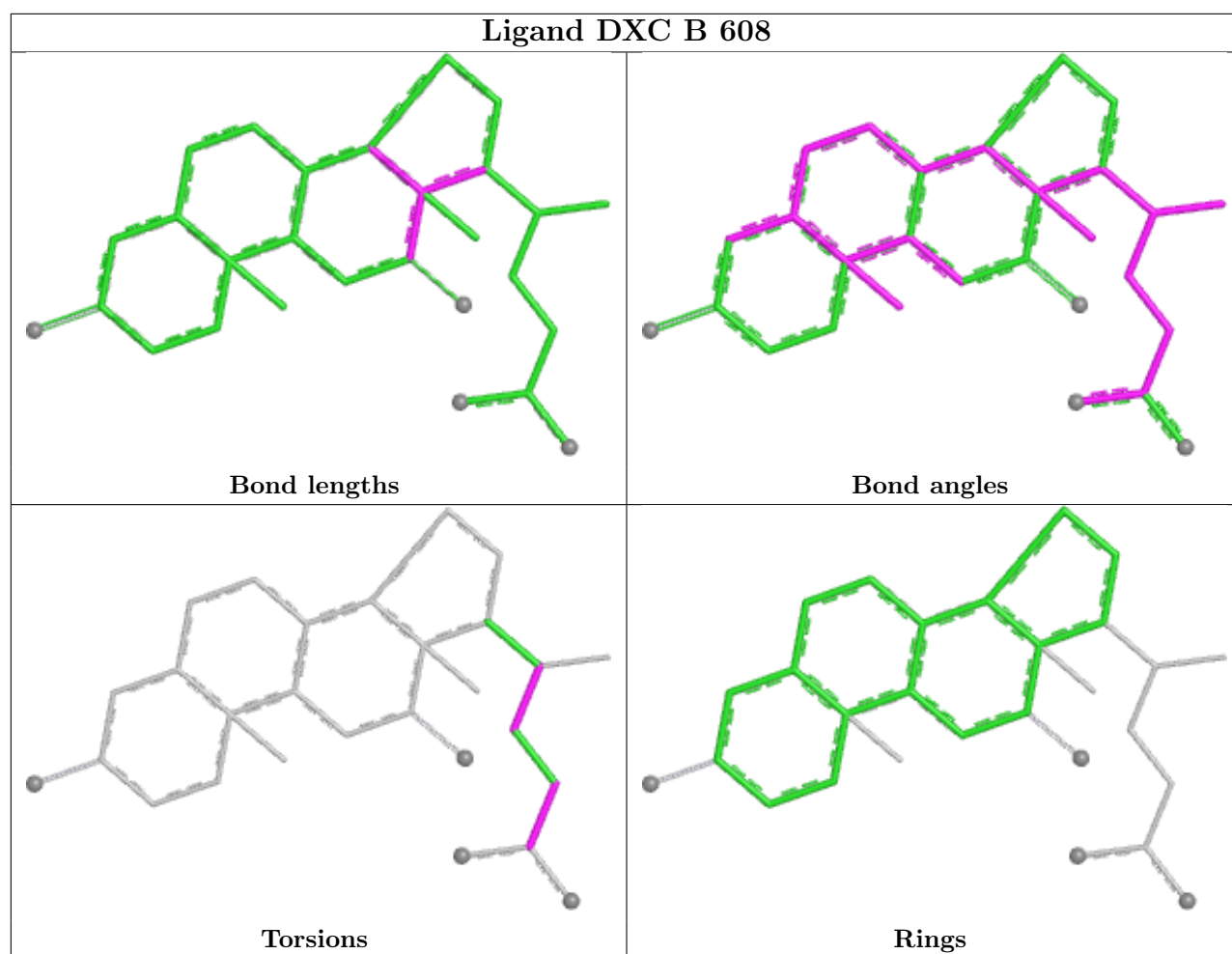


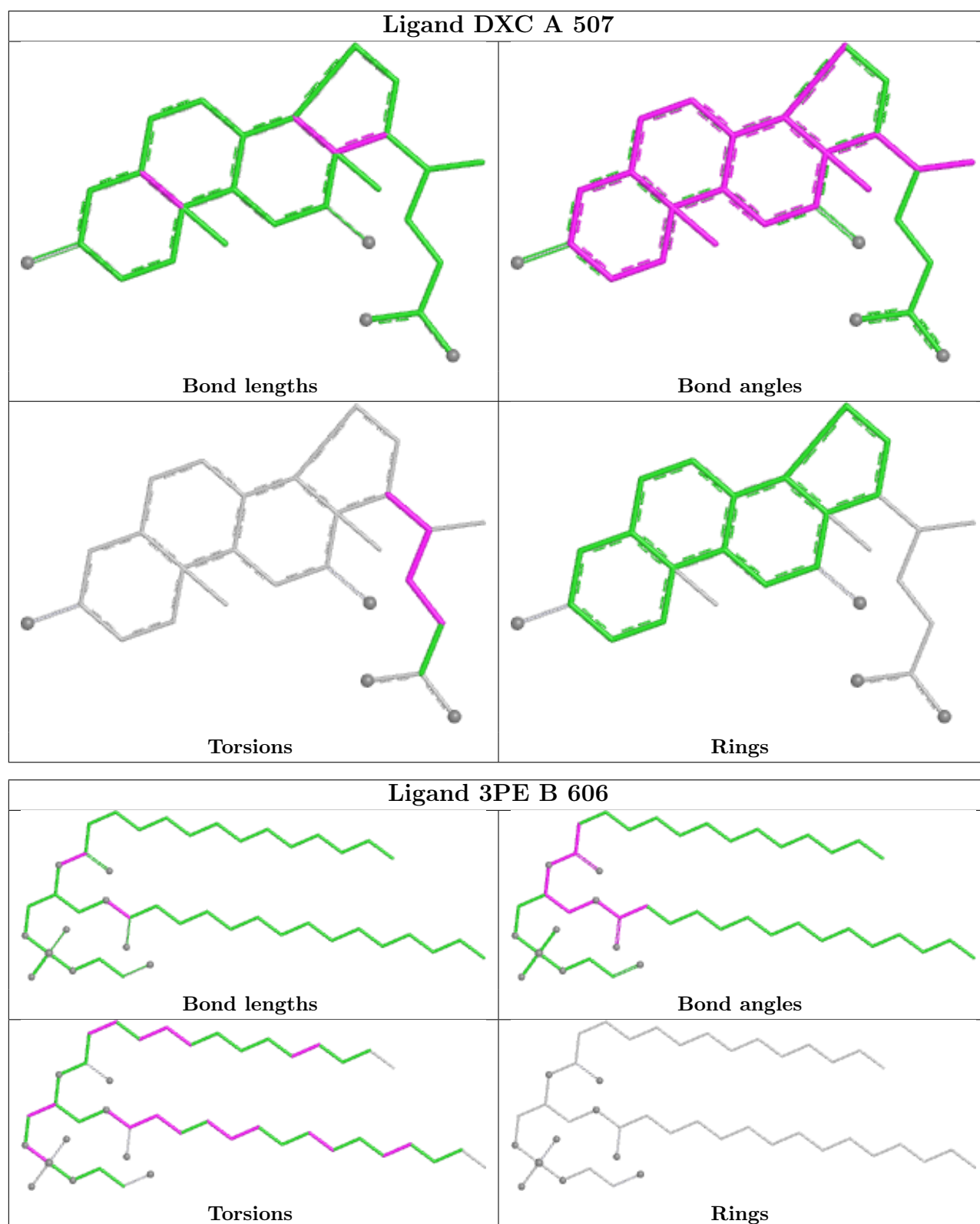
Ligand 3PE A 503











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	321/393 (81%)	0.66	40 (12%) 8 6	38, 81, 135, 166	8 (2%)
1	B	322/393 (81%)	0.31	29 (9%) 15 12	21, 62, 110, 134	7 (2%)
All	All	643/786 (81%)	0.48	69 (10%) 11 9	21, 71, 125, 166	15 (2%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178[A]	ILE	10.7
1	B	178[A]	ILE	8.9
1	B	62	ASP	7.5
1	B	72	TRP	6.7
1	A	62	ASP	6.2
1	B	120	VAL	5.6
1	B	77	ILE	4.9
1	A	72	TRP	4.8
1	B	119	GLY	4.6
1	A	93	VAL	4.5
1	A	120	VAL	4.4
1	A	77	ILE	4.3
1	B	117	GLU	4.2
1	B	179[A]	ASP	4.2
1	A	78	PRO	3.9
1	A	264[A]	LYS	3.7
1	B	61	LYS	3.6
1	B	66	VAL	3.4
1	A	273	LEU	3.4
1	B	65	PHE	3.3
1	B	73	LYS	3.3
1	A	73	LYS	3.3
1	B	60	GLY	3.2
1	B	124	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	93	VAL	3.1
1	A	232	TRP	3.1
1	A	265	VAL	3.1
1	A	94	PRO	3.0
1	B	122	GLU	3.0
1	B	121	ARG	3.0
1	B	118	ALA	3.0
1	B	94	PRO	2.9
1	B	59	LYS	2.9
1	B	78	PRO	2.9
1	A	63	GLY	2.8
1	A	260	MET	2.8
1	A	60	GLY	2.7
1	A	65	PHE	2.7
1	A	71	THR	2.7
1	A	79	ASN	2.7
1	A	95	SER	2.6
1	A	74	ASN	2.6
1	B	69	TRP	2.6
1	A	118	ALA	2.6
1	A	144	PHE	2.6
1	A	66	VAL	2.6
1	B	71	THR	2.5
1	A	121	ARG	2.5
1	A	298	PHE	2.5
1	A	287	TYR	2.5
1	A	246	PHE	2.5
1	A	215	LEU	2.4
1	A	119	GLY	2.4
1	B	232	TRP	2.4
1	A	286	GLY	2.4
1	A	96	SER	2.4
1	B	63	GLY	2.3
1	B	79	ASN	2.3
1	B	75	PRO	2.3
1	A	367	ARG	2.2
1	B	57	SER	2.2
1	A	122	GLU	2.2
1	A	315	TRP	2.1
1	A	388	ASN	2.1
1	A	58	LYS	2.1
1	A	179[A]	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	91	SER	2.1
1	A	69	TRP	2.0
1	A	204	GLY	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](#)

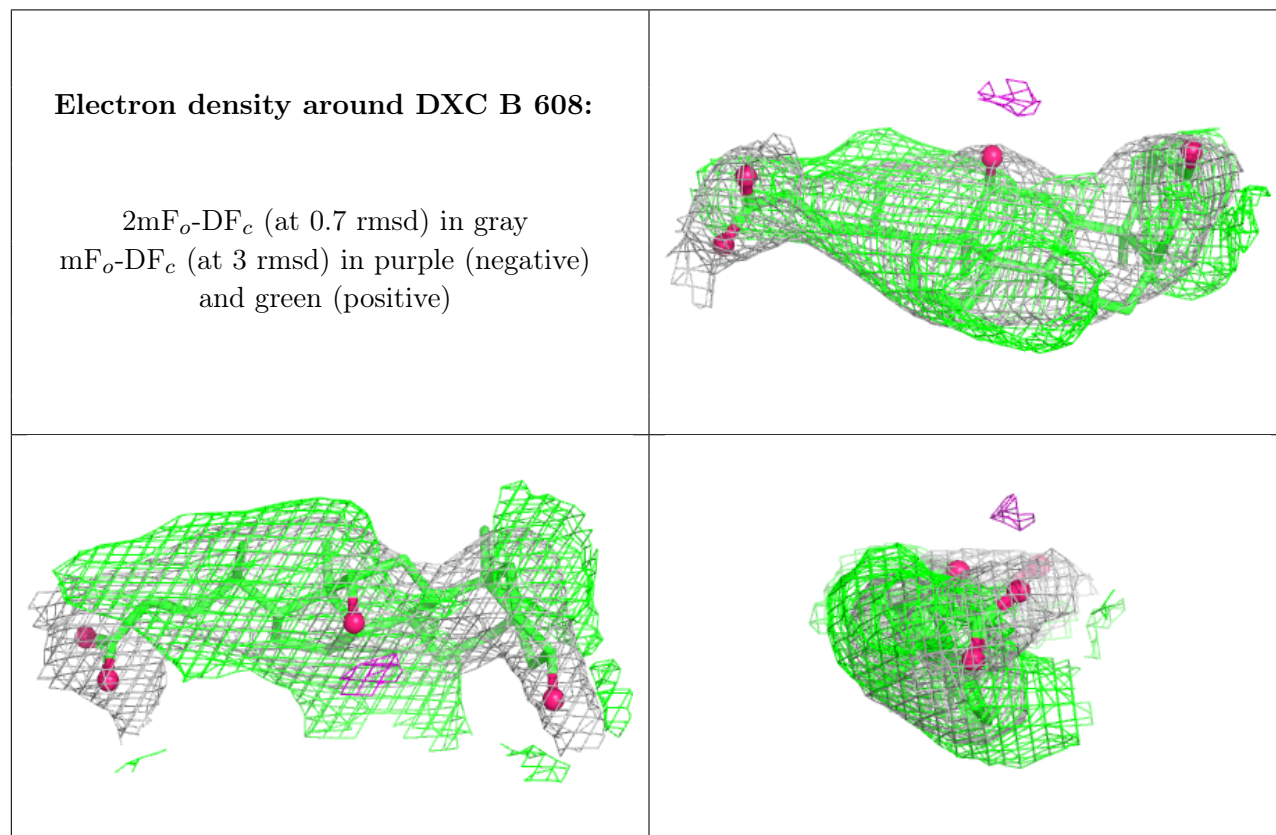
There are no oligosaccharides in this entry.

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.

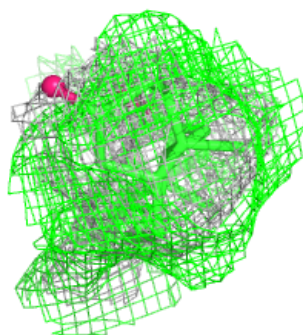
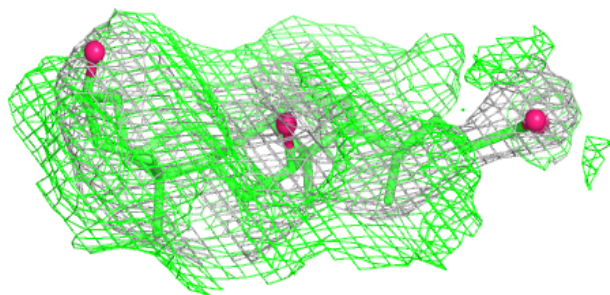
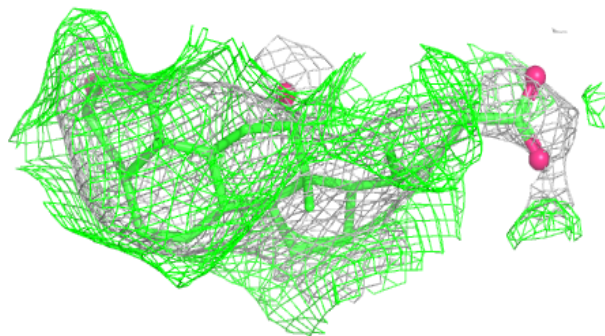
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	A	509	5/5	0.76	0.24	53,63,73,74	5
5	SO4	A	508	5/5	0.80	0.19	52,57,63,73	5
4	DXC	B	608	28/28	0.84	0.36	44,58,69,69	28
4	DXC	B	610	28/28	0.84	0.47	67,76,81,85	28
4	DXC	B	609	28/28	0.86	0.35	49,56,72,75	28
5	SO4	B	611	5/5	0.87	0.13	44,52,57,63	5
4	DXC	A	507	28/28	0.88	0.22	73,83,88,89	28
4	DXC	B	603	28/28	0.89	0.20	66,74,82,84	28
3	3PE	A	503	44/51	0.94	0.15	58,69,80,98	0
4	DXC	B	601	28/28	0.94	0.12	55,71,79,80	0
4	DXC	A	504	28/28	0.94	0.11	63,67,95,100	0
4	DXC	B	607	28/28	0.94	0.14	61,69,73,76	0
4	DXC	A	506	28/28	0.94	0.11	55,64,75,90	0
4	DXC	A	505	28/28	0.95	0.09	50,54,78,86	0
4	DXC	B	602	28/28	0.95	0.12	64,73,82,88	0
3	3PE	B	606	44/51	0.96	0.14	53,68,81,93	0
2	ZN	A	501	1/1	0.99	0.04	64,64,64,64	0
2	ZN	A	502	1/1	0.99	0.04	66,66,66,66	0
2	ZN	B	604	1/1	0.99	0.07	60,60,60,60	0
2	ZN	B	605	1/1	0.99	0.04	58,58,58,58	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.

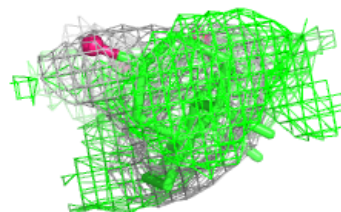
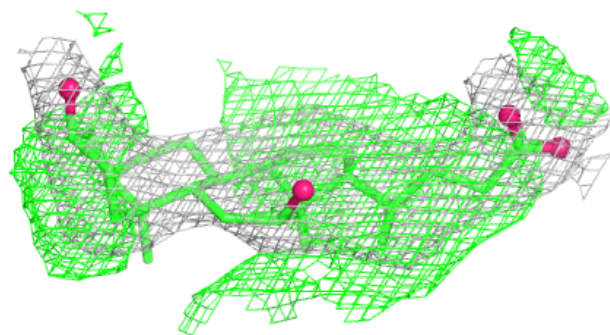
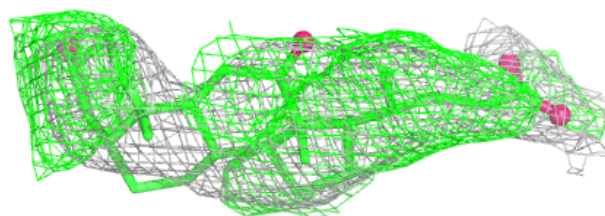


Electron density around DXC B 610:

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

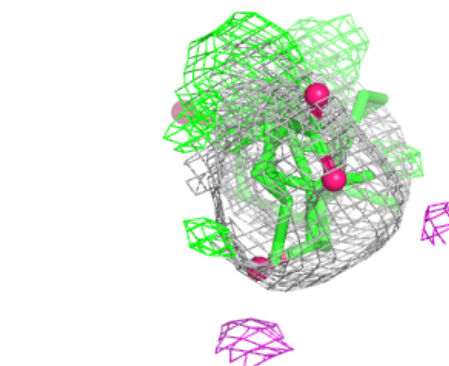
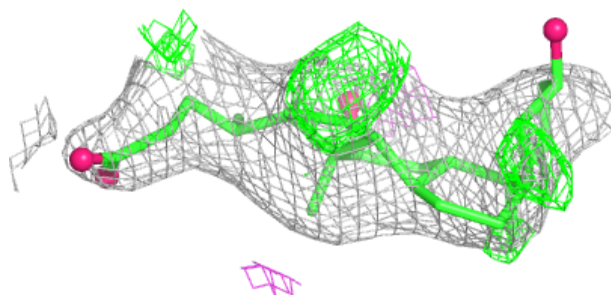
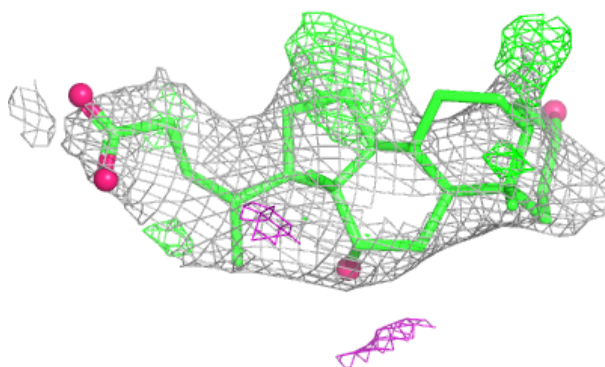
**Electron density around DXC B 609:**

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

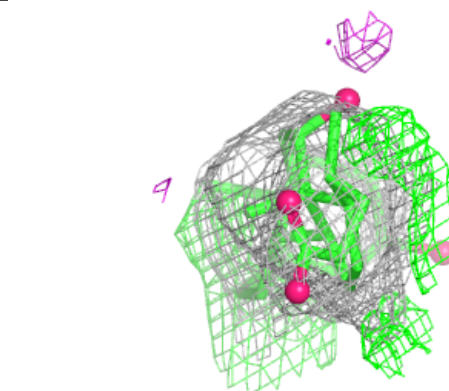
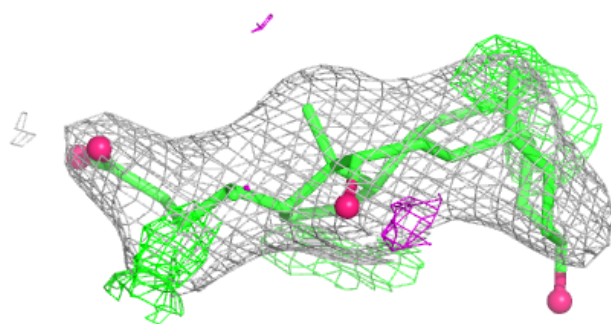
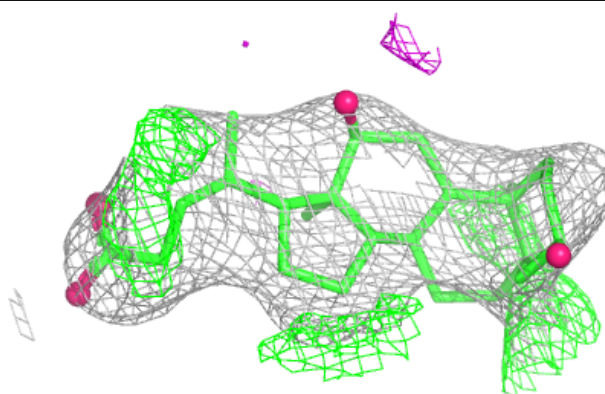


Electron density around DXC A 507:

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

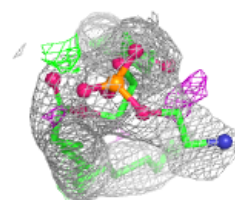
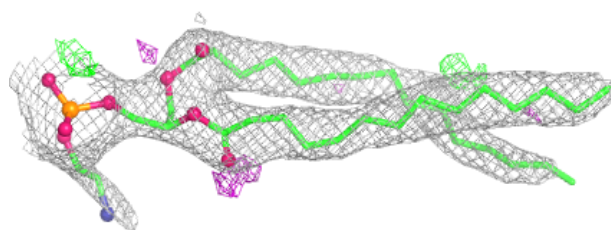
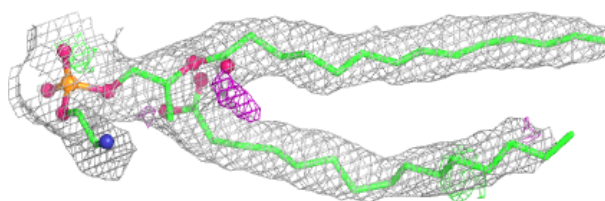
**Electron density around DXC B 603:**

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

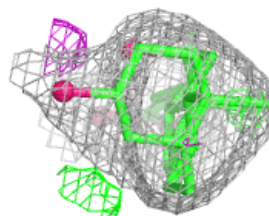
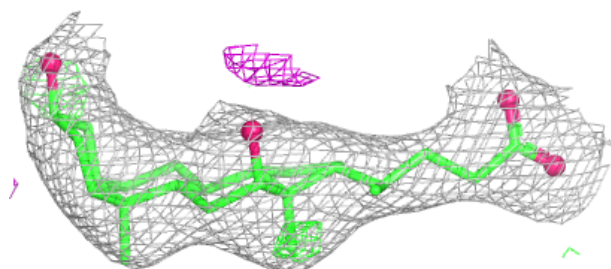
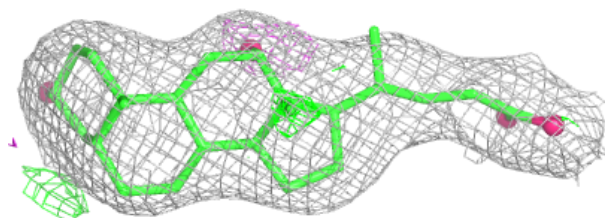


Electron density around 3PE A 503:

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

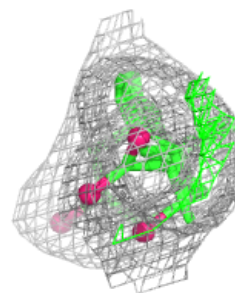
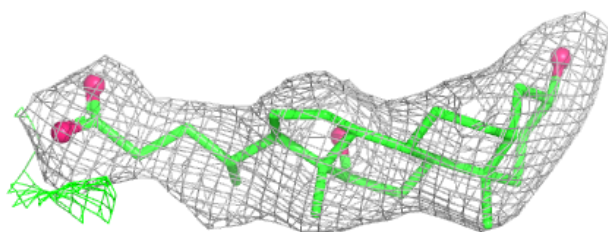
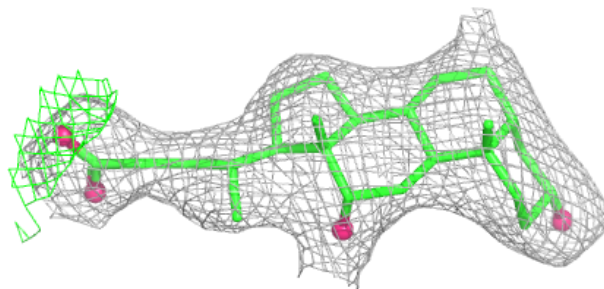
**Electron density around DXC B 601:**

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

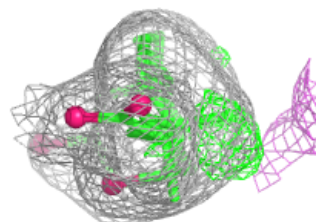
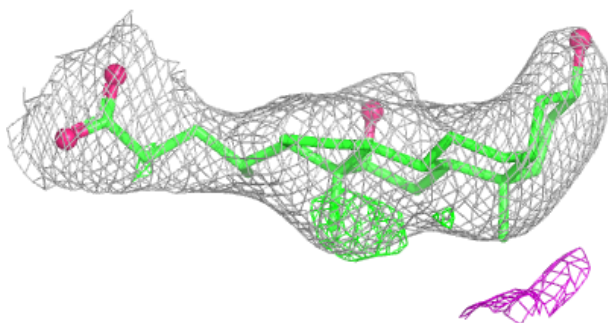
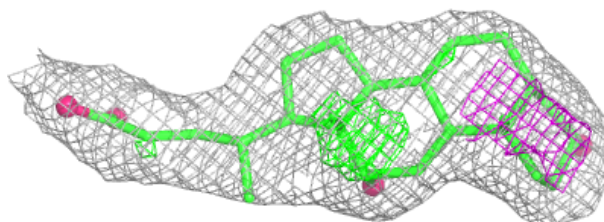


Electron density around DXC A 504:

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

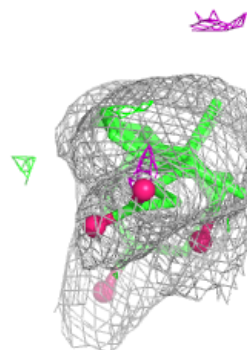
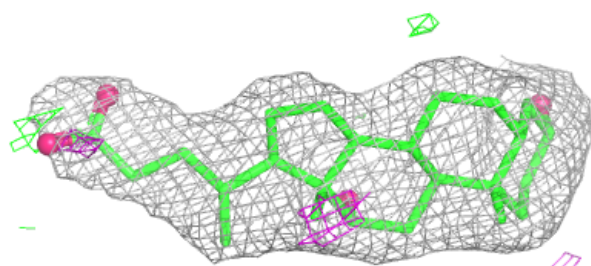
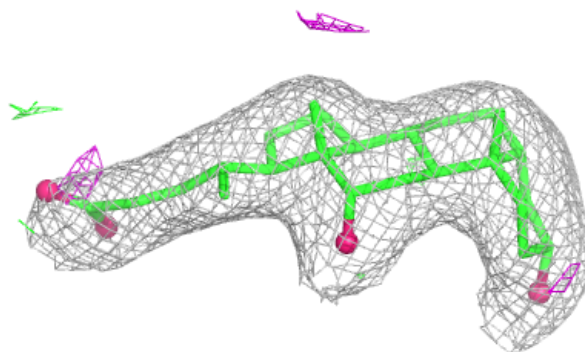
**Electron density around DXC B 607:**

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

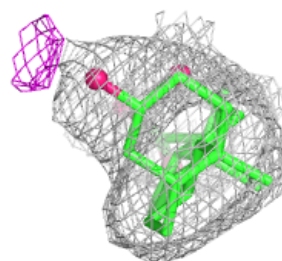
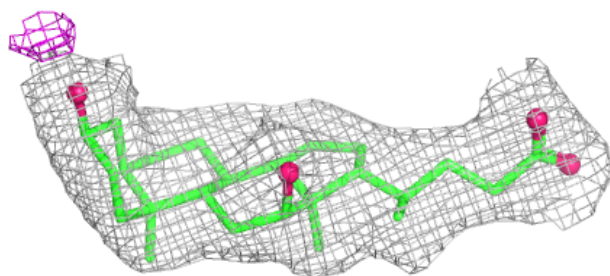
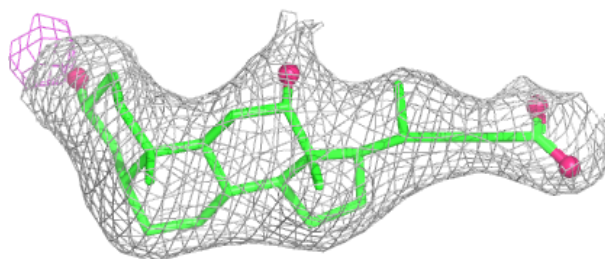


Electron density around DXC A 506:

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

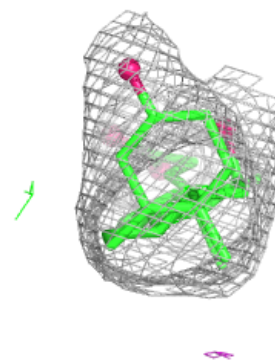
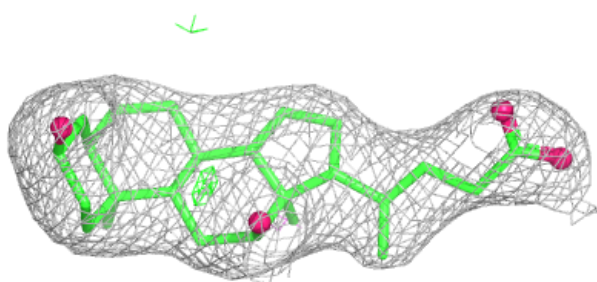
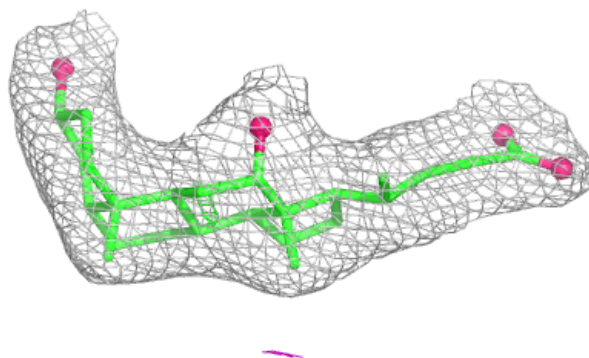
**Electron density around DXC A 505:**

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

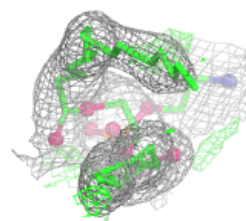
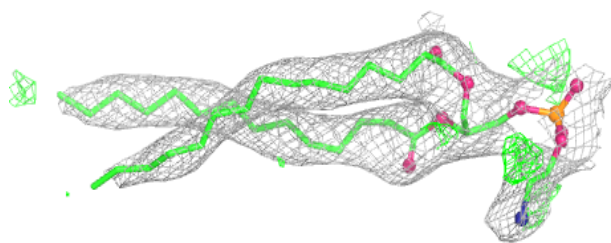
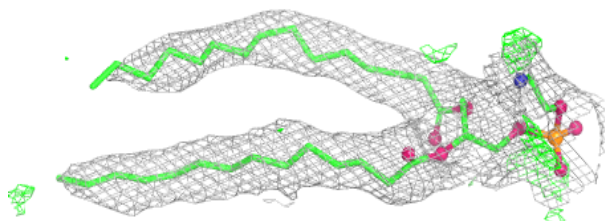


Electron density around DXC B 602:

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

**Electron density around 3PE B 606:**

$2mF_o-DF_c$ (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.