Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 08:03 AM EDT

PDB ID	:	7L92
Title	:	C1B domain of Protein kinase C in complex with diacylglycerol and dodecyl 2-(trimethylammonio)ethyl phosphate
Authors	:	Katti, S.S.; Krieger, I.V.
Deposited on	:	2021-01-01
Resolution	:	1.75 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:

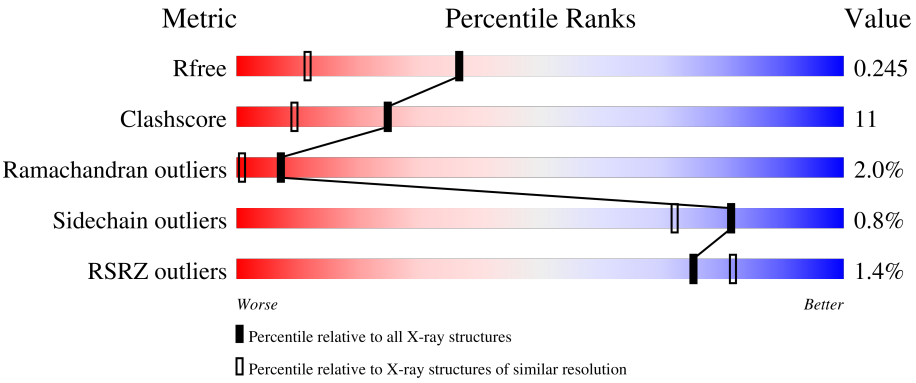
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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	53	70% 26%
1	D	53	4% 77% 19%
1	G	53	2% 85% 11%
1	J	53	4% 81% 13%
1	M	53	2% 81% 17%

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Mol	Chain	Length	Quality of chain
1	P	53	77% 19%
1	S	53	75% 23%
1	V	53	85% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EOH	A	305	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4042 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 Protein kinase C delta type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	52	Total	C	N	O	S	0	2	0
			426	270	76	69	11			
1	D	51	Total	C	N	O	S	0	1	0
			413	261	75	68	9			
1	G	52	Total	C	N	O	S	0	2	0
			429	271	79	69	10			
1	J	51	Total	C	N	O	S	0	1	0
			413	261	75	68	9			
1	M	52	Total	C	N	O	S	0	1	0
			421	266	76	69	10			
1	P	52	Total	C	N	O	S	0	1	0
			420	266	76	69	9			
1	S	52	Total	C	N	O	S	0	0	0
			416	262	76	69	9			
1	V	52	Total	C	N	O	S	0	2	0
			426	271	76	69	10			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	G	2	Total	Zn	0	0
			2	2		
2	J	2	Total	Zn	0	0
			2	2		
2	M	2	Total	Zn	0	0
			2	2		
2	P	2	Total	Zn	0	0
			2	2		

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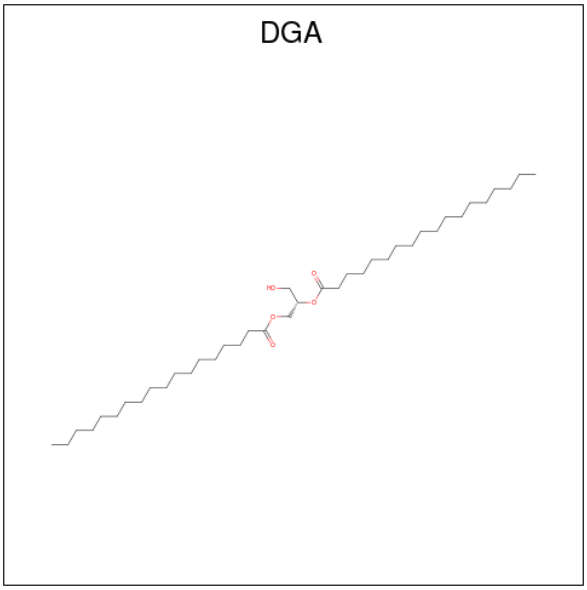
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	S	2	Total Zn 2 2	0	0
2	V	2	Total Zn 2 2	0	0

- Molecule 3 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 48 38 10	0	1
3	A	1	Total C O 24 19 5	0	0
3	D	1	Total C O 24 19 5	0	0
3	G	1	Total C O 24 19 5	0	0
3	G	1	Total C O 24 19 5	0	0
3	J	1	Total C O 24 19 5	0	0
3	M	1	Total C O 24 19 5	0	0
3	P	1	Total C O 24 19 5	0	0
3	S	1	Total C O 24 19 5	0	0

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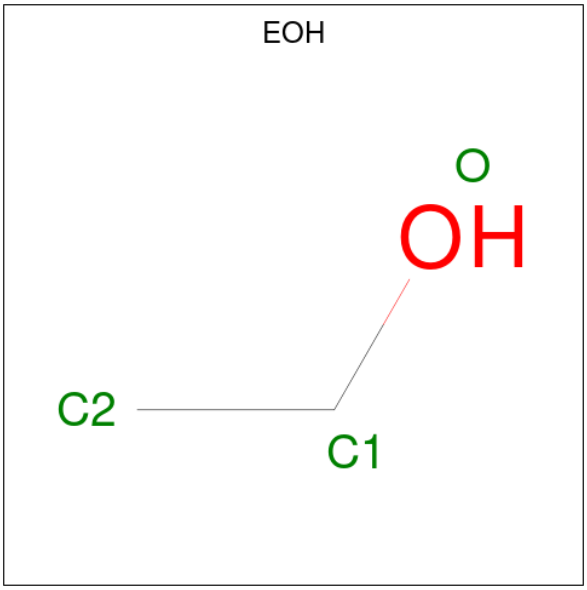
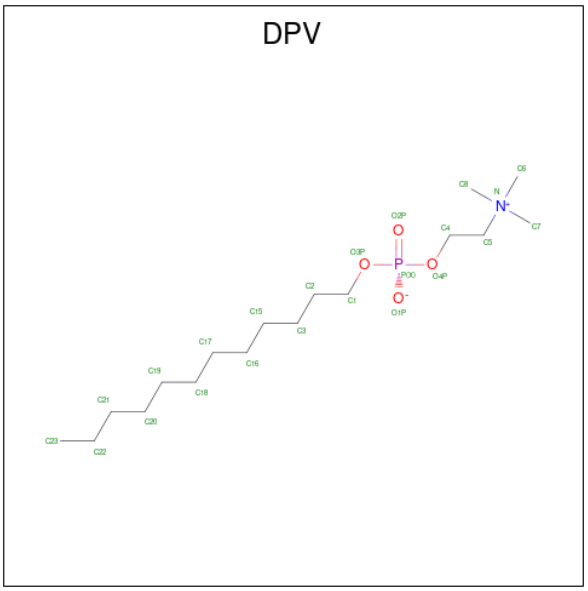
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	V	1	Total C O 24 19 5	0	0

- Molecule 4 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 2 1	0	0
4	S	1	Total C O 3 2 1	0	0

- Molecule 5 is dodecyl 2-(trimethylammonio)ethyl phosphate (three-letter code: DPV) (formula: $C_{17}H_{38}NO_4P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			23	17	1	4	1		
5	J	1	Total	C	N	O	P	0	0
			23	17	1	4	1		
5	M	1	Total	C	N	O	P	0	1
			46	34	2	8	2		
5	P	1	Total	C	N	O	P	0	0
			23	17	1	4	1		
5	S	1	Total	C	N	O	P	0	0
			23	17	1	4	1		
5	V	1	Total	C	N	O	P	0	0
			23	17	1	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	21	Total	O	0	0
			21	21		
6	D	32	Total	O	0	0
			32	32		
6	G	24	Total	O	0	0
			24	24		
6	J	36	Total	O	0	0
			36	36		
6	M	37	Total	O	0	0
			37	37		
6	P	18	Total	O	0	0
			18	18		

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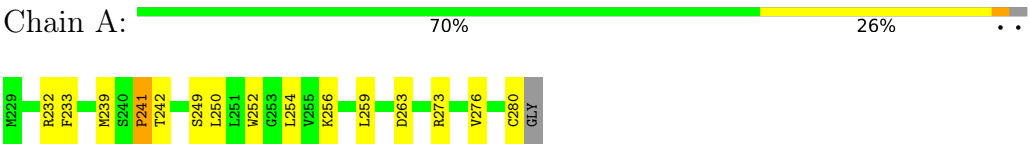
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	S	30	Total O 30 30	0	0
6	V	33	Total O 33 33	0	0

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.

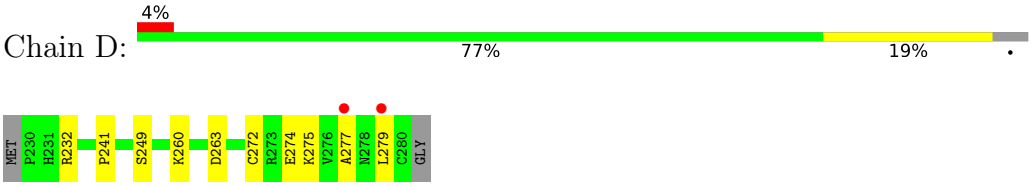
• Molecule 1: Protein kinase C delta type

Chain A:



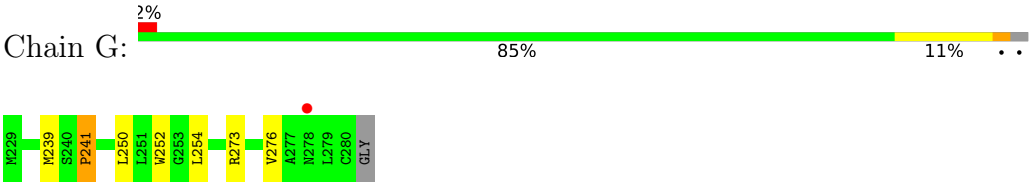
• Molecule 1: Protein kinase C delta type

Chain D:



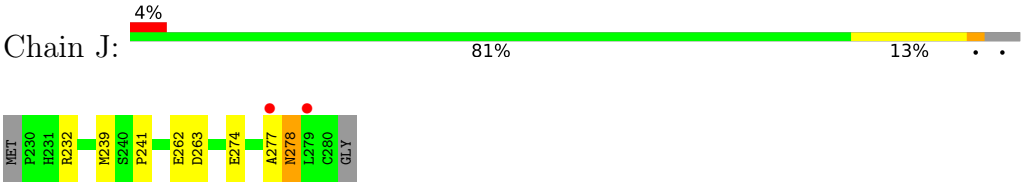
• Molecule 1: Protein kinase C delta type

Chain G:



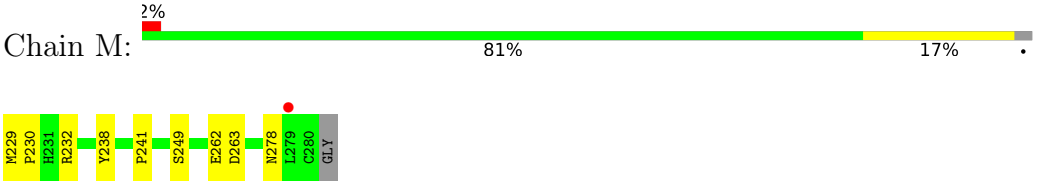
• Molecule 1: Protein kinase C delta type

Chain J:



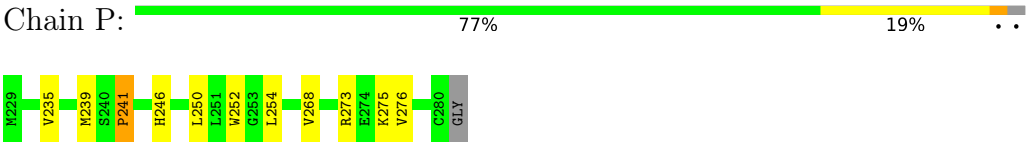
• Molecule 1: Protein kinase C delta type

Chain M:



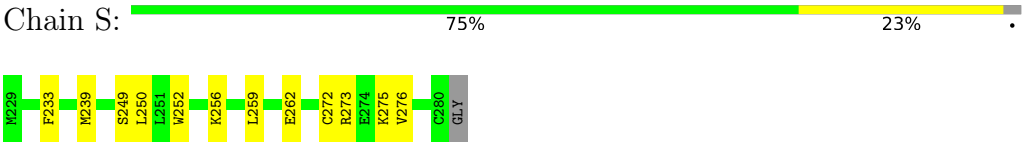
• Molecule 1: Protein kinase C delta type

Chain P:



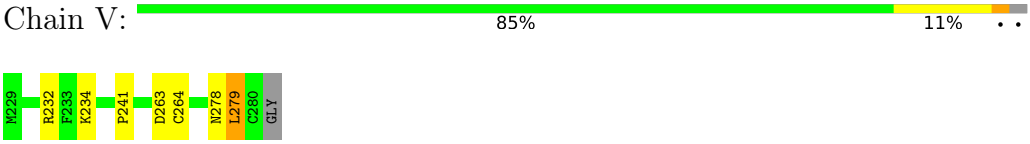
• Molecule 1: Protein kinase C delta type

Chain S:



• Molecule 1: Protein kinase C delta type

Chain V:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	89.07Å 89.07Å 218.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.96 – 1.75 44.60 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.96-1.75) 95.6 (44.60-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.214 , 0.246 0.215 , 0.245	Depositor DCC
R_{free} test set	3398 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 20.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.145 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.149 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.148 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.469 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.469 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.470 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.149 for -h-k,k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4042	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: DGA, EOH, DPV, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.44	0/443	0.67	0/593
1	D	0.48	0/427	0.70	0/571
1	G	0.39	0/446	0.58	0/596
1	J	0.45	0/427	0.69	0/571
1	M	0.46	0/435	0.67	0/582
1	P	0.44	0/434	0.69	0/582
1	S	0.41	0/427	0.61	0/572
1	V	0.44	0/443	0.67	0/593
All	All	0.44	0/3482	0.66	0/4660

There are no bond length outliers.

There are no bond angle outliers.

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	426	0	417	13	0
1	D	413	0	401	7	0
1	G	429	0	422	7	0
1	J	413	0	401	6	0
1	M	421	0	409	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	420	0	409	13	0
1	S	416	0	400	9	0
1	V	426	0	420	6	0
2	A	2	0	0	0	0
2	D	2	0	0	0	0
2	G	2	0	0	0	0
2	J	2	0	0	0	0
2	M	2	0	0	0	0
2	P	2	0	0	0	0
2	S	2	0	0	0	0
2	V	2	0	0	0	0
3	A	72	0	90	2	0
3	D	24	0	30	1	0
3	G	48	0	60	7	0
3	J	24	0	30	2	0
3	M	24	0	30	5	0
3	P	24	0	30	5	0
3	S	24	0	30	0	0
3	V	24	0	30	0	0
4	A	3	0	6	3	0
4	S	3	0	6	1	0
5	D	23	0	38	3	0
5	J	23	0	38	1	0
5	M	46	0	76	7	0
5	P	23	0	38	2	0
5	S	23	0	38	2	0
5	V	23	0	38	3	0
6	A	21	0	0	4	0
6	D	32	0	0	3	0
6	G	24	0	0	0	0
6	J	36	0	0	2	0
6	M	37	0	0	1	0
6	P	18	0	0	0	0
6	S	30	0	0	1	0
6	V	33	0	0	0	0
All	All	4042	0	3887	83	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 11.

All (83) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:CYS:SG	6:A:412:HOH:O	2.28	0.92
1:P:250:LEU:HD22	5:P:304:DPV:H8B	1.70	0.74
1:D:241:PRO:HG2	5:D:304:DPV:H2A	1.74	0.70
3:M:303:DGA:HA71	5:M:304[B]:DPV:H22A	1.75	0.69
1:S:249:SER:HA	5:S:304:DPV:H2	1.80	0.64
1:G:241:PRO:HA	3:G:303:DGA:HG32	1.78	0.63
1:G:239[B]:MET:HA	3:G:303:DGA:HA21	1.81	0.63
1:J:232:ARG:NH2	1:J:262:GLU:OE1	2.32	0.63
1:P:241:PRO:HA	3:P:303:DGA:HG32	1.83	0.61
1:V:278:ASN:O	1:V:279:LEU:HB2	1.99	0.61
1:D:232:ARG:NH1	1:D:263:ASP:OD1	2.35	0.60
1:A:241:PRO:HB3	6:A:421:HOH:O	2.01	0.59
1:A:232:ARG:NH2	6:A:401:HOH:O	2.25	0.59
5:M:304[A]:DPV:H2A	1:V:241:PRO:HG2	1.83	0.59
1:P:254:LEU:HD21	3:P:303:DGA:HB71	1.87	0.57
1:S:250:LEU:HD22	5:S:304:DPV:H7B	1.86	0.57
1:A:232:ARG:HD3	1:A:263:ASP:OD2	2.05	0.57
1:M:241:PRO:CG	5:M:304[A]:DPV:H18	2.35	0.57
5:V:304:DPV:H17	5:V:304:DPV:H1	1.87	0.57
3:G:304:DGA:HG2	3:G:304:DGA:HA32	1.86	0.55
1:P:246:HIS:NE2	1:P:275:LYS:HE2	2.21	0.55
1:P:254:LEU:HD22	3:P:303:DGA:HA61	1.90	0.54
1:J:232:ARG:NH1	1:J:263:ASP:OD2	2.41	0.54
1:P:273:ARG:O	1:P:276[B]:VAL:HG22	2.08	0.53
1:J:274:GLU:HG2	6:J:401:HOH:O	2.09	0.53
1:P:252:TRP:HB3	1:S:252:TRP:HB3	1.91	0.52
1:A:233:PHE:O	4:A:305:EOH:H21	2.10	0.52
1:M:229:MET:N	1:M:230:PRO:HD2	2.23	0.52
5:J:304:DPV:H6A	5:J:304:DPV:O2P	2.10	0.51
1:M:229:MET:N	1:M:229:MET:SD	2.84	0.50
4:A:305:EOH:H23	1:D:260:LYS:HE3	1.93	0.50
5:V:304:DPV:O1P	5:V:304:DPV:H2	2.11	0.50
1:M:241:PRO:HG3	5:M:304[A]:DPV:H20	1.93	0.50
1:G:239[A]:MET:HA	3:G:303:DGA:HA21	1.94	0.49
1:P:239:MET:HA	3:P:303:DGA:HA21	1.93	0.49
1:A:252:TRP:HB3	1:G:252:TRP:HB3	1.93	0.49
1:M:249:SER:HB3	6:M:411:HOH:O	2.13	0.49
1:D:274:GLU:OE2	1:D:274:GLU:HA	2.12	0.49
1:P:235:VAL:HG21	1:V:264:CYS:HB2	1.95	0.48
1:G:250:LEU:HB2	3:G:304:DGA:HG12	1.96	0.48
3:M:303:DGA:HB61	5:M:304[A]:DPV:H22A	1.94	0.48
1:S:273:ARG:O	1:S:276:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:241:PRO:HG3	5:M:304[A]:DPV:H18	1.96	0.47
5:P:304:DPV:H8A	5:P:304:DPV:H4	1.62	0.47
1:A:256:LYS:HE2	6:D:425:HOH:O	2.15	0.47
1:S:262:GLU:HA	4:S:305:EOH:H22	1.96	0.47
1:D:249:SER:HB3	6:D:410:HOH:O	2.13	0.47
1:J:239[A]:MET:HE1	6:J:429:HOH:O	2.15	0.46
3:D:303:DGA:HA31	3:D:303:DGA:HB61	1.97	0.46
1:M:232:ARG:NH1	1:M:263:ASP:OD1	2.48	0.46
1:S:233:PHE:HB3	1:S:259:LEU:HB3	1.98	0.46
3:M:303:DGA:HA62	3:M:303:DGA:HA31	1.67	0.46
1:S:256:LYS:NZ	6:S:402:HOH:O	2.48	0.45
1:J:277:ALA:O	1:J:278:ASN:OD1	2.35	0.45
1:P:268:VAL:HG11	1:P:276[A]:VAL:HG21	1.99	0.45
1:A:254:LEU:HD22	3:A:303[A]:DGA:HB41	1.99	0.44
1:A:273:ARG:NH1	1:A:273:ARG:HB3	2.32	0.44
1:A:249:SER:HB3	6:A:404:HOH:O	2.17	0.44
1:M:238:TYR:O	3:M:303:DGA:HB22	2.18	0.44
5:D:304:DPV:H20A	5:D:304:DPV:H23A	1.72	0.44
1:D:272:CYS:HA	1:D:275:LYS:HD3	1.99	0.44
1:V:232:ARG:NH1	1:V:263:ASP:OD2	2.50	0.44
1:G:254:LEU:HD22	3:G:303:DGA:HA62	2.00	0.43
1:M:229:MET:N	1:M:230:PRO:CD	2.80	0.43
3:J:303:DGA:HA32	3:J:303:DGA:HA62	1.65	0.43
1:S:272:CYS:HA	1:S:275:LYS:HD3	2.00	0.43
1:V:234:LYS:HE2	1:V:234:LYS:HB3	1.79	0.43
3:M:303:DGA:HB61	5:M:304[A]:DPV:H20A	2.01	0.42
1:P:235:VAL:CG2	1:V:264:CYS:HB2	2.49	0.42
3:G:304:DGA:HB51	3:G:304:DGA:HB21	1.72	0.42
5:V:304:DPV:H8A	5:V:304:DPV:H4	1.55	0.42
4:A:305:EOH:H23	1:D:260:LYS:CE	2.48	0.42
1:A:233:PHE:HB3	1:A:259:LEU:HB3	2.02	0.42
1:M:230:PRO:HA	1:M:278:ASN:HA	2.00	0.42
1:A:273:ARG:O	1:A:276:VAL:HG22	2.20	0.42
1:J:241:PRO:HA	3:J:303:DGA:HG2	2.01	0.42
5:D:304:DPV:H15	6:D:432:HOH:O	2.19	0.41
1:P:241:PRO:HA	3:P:303:DGA:CG3	2.48	0.41
1:A:242:THR:O	1:A:250:LEU:HD12	2.20	0.40
1:P:268:VAL:HG11	1:P:276[B]:VAL:HG11	2.03	0.40
1:S:273:ARG:HB3	1:S:273:ARG:NH1	2.36	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	51/53 (96%)	50 (98%)	0	1 (2%)	7 1
1	D	50/53 (94%)	45 (90%)	3 (6%)	2 (4%)	3 0
1	G	52/53 (98%)	50 (96%)	1 (2%)	1 (2%)	8 1
1	J	50/53 (94%)	47 (94%)	2 (4%)	1 (2%)	7 1
1	M	51/53 (96%)	47 (92%)	3 (6%)	1 (2%)	7 1
1	P	51/53 (96%)	48 (94%)	2 (4%)	1 (2%)	7 1
1	S	50/53 (94%)	48 (96%)	2 (4%)	0	100 100
1	V	52/53 (98%)	46 (88%)	5 (10%)	1 (2%)	8 1
All	All	407/424 (96%)	381 (94%)	18 (4%)	8 (2%)	7 1

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	279	LEU
1	V	279	LEU
1	D	277	ALA
1	G	241	PRO
1	J	278	ASN
1	M	262	GLU
1	P	241	PRO
1	A	241	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	49/47 (104%)	47 (96%)	2 (4%)	30 10
1	D	47/47 (100%)	47 (100%)	0	100 100
1	G	49/47 (104%)	47 (96%)	2 (4%)	30 10
1	J	47/47 (100%)	47 (100%)	0	100 100
1	M	48/47 (102%)	48 (100%)	0	100 100
1	P	48/47 (102%)	48 (100%)	0	100 100
1	S	47/47 (100%)	46 (98%)	1 (2%)	53 31
1	V	49/47 (104%)	49 (100%)	0	100 100
All	All	384/376 (102%)	379 (99%)	5 (1%)	81 54

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239[A]	MET
1	A	239[B]	MET
1	G	273[A]	ARG
1	G	273[B]	ARG
1	S	239	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 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	DGA	S	303	-	23,23,43	1.37	2 (8%)	25,25,45	1.72	5 (20%)
3	DGA	V	303	-	23,23,43	1.12	2 (8%)	25,25,45	1.26	4 (16%)
5	DPV	M	304[B]	-	22,22,22	0.91	0	26,27,27	0.60	0
4	EOH	S	305	-	2,2,2	0.45	0	1,1,1	0.55	0
3	DGA	G	303	-	23,23,43	1.35	2 (8%)	25,25,45	1.47	5 (20%)
4	EOH	A	305	-	2,2,2	0.47	0	1,1,1	0.25	0
3	DGA	A	303[A]	-	23,23,43	1.30	2 (8%)	25,25,45	1.32	4 (16%)
3	DGA	P	303	-	23,23,43	1.30	2 (8%)	25,25,45	1.48	5 (20%)
5	DPV	J	304	-	22,22,22	0.88	0	26,27,27	0.65	1 (3%)
5	DPV	P	304	-	22,22,22	0.95	0	26,27,27	0.43	0
3	DGA	J	303	-	23,23,43	1.12	2 (8%)	25,25,45	1.18	3 (12%)
5	DPV	S	304	-	22,22,22	0.90	0	26,27,27	0.49	0
3	DGA	M	303	-	23,23,43	1.09	2 (8%)	25,25,45	1.42	3 (12%)
3	DGA	D	303	-	23,23,43	1.09	2 (8%)	25,25,45	1.28	4 (16%)
5	DPV	M	304[A]	-	22,22,22	0.88	0	26,27,27	0.60	0
3	DGA	G	304	-	23,23,43	1.38	2 (8%)	25,25,45	1.61	4 (16%)
3	DGA	A	303[B]	-	23,23,43	1.28	2 (8%)	25,25,45	1.28	3 (12%)
3	DGA	A	304	-	23,23,43	1.33	2 (8%)	25,25,45	1.47	4 (16%)
5	DPV	V	304	-	22,22,22	0.95	0	26,27,27	0.69	0
5	DPV	D	304	-	22,22,22	0.92	0	26,27,27	0.68	0

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	DGA	S	303	-	-	10/25/25/45	-
3	DGA	V	303	-	-	9/25/25/45	-
3	DGA	A	303[A]	-	-	10/25/25/45	-
5	DPV	M	304[B]	-	-	13/22/22/22	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DPV	V	304	-	-	10/22/22/22	-
5	DPV	P	304	-	-	11/22/22/22	-
3	DGA	J	303	-	-	7/25/25/45	-
3	DGA	G	303	-	-	9/25/25/45	-
5	DPV	S	304	-	-	13/22/22/22	-
5	DPV	D	304	-	-	11/22/22/22	-
3	DGA	P	303	-	-	11/25/25/45	-
3	DGA	M	303	-	-	10/25/25/45	-
3	DGA	D	303	-	-	8/25/25/45	-
5	DPV	M	304[A]	-	-	14/22/22/22	-
3	DGA	G	304	-	-	14/25/25/45	-
3	DGA	A	303[B]	-	-	10/25/25/45	-
5	DPV	J	304	-	-	12/22/22/22	-
3	DGA	A	304	-	-	15/25/25/45	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	303	DGA	OG2-CB1	4.55	1.47	1.34
3	S	303	DGA	OG1-CA1	4.50	1.46	1.33
3	G	304	DGA	OG2-CB1	4.45	1.46	1.34
3	G	304	DGA	OG1-CA1	4.38	1.46	1.33
3	A	304	DGA	OG1-CA1	4.36	1.46	1.33
3	P	303	DGA	OG2-CB1	4.25	1.46	1.34
3	A	303[A]	DGA	OG1-CA1	4.21	1.45	1.33
3	A	303[B]	DGA	OG1-CA1	4.17	1.45	1.33
3	A	304	DGA	OG2-CB1	4.12	1.45	1.34
3	P	303	DGA	OG1-CA1	4.06	1.45	1.33
3	G	303	DGA	OG1-CA1	3.99	1.45	1.33
3	A	303[A]	DGA	OG2-CB1	3.96	1.45	1.34
3	S	303	DGA	OG2-CB1	3.92	1.45	1.34
3	A	303[B]	DGA	OG2-CB1	3.86	1.45	1.34
3	V	303	DGA	OG1-CA1	3.84	1.44	1.33
3	D	303	DGA	OG1-CA1	3.82	1.44	1.33
3	J	303	DGA	OG1-CA1	3.70	1.44	1.33
3	M	303	DGA	OG1-CA1	3.60	1.43	1.33
3	J	303	DGA	OG2-CB1	3.05	1.42	1.34
3	V	303	DGA	OG2-CB1	2.74	1.42	1.34
3	M	303	DGA	OG2-CB1	2.68	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	303	DGA	OG2-CB1	2.50	1.41	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	304	DGA	OG2-CB1-CB2	5.49	123.33	111.50
3	A	304	DGA	OG2-CB1-CB2	4.61	121.43	111.50
3	P	303	DGA	OG2-CB1-CB2	4.42	121.03	111.50
3	G	303	DGA	OG2-CB1-CB2	4.21	120.58	111.50
3	S	303	DGA	CG2-OG2-CB1	-4.01	107.91	117.79
3	A	303[A]	DGA	OG2-CB1-CB2	3.82	119.74	111.50
3	S	303	DGA	OG1-CA1-CA2	3.82	123.89	111.91
3	S	303	DGA	OG2-CB1-CB2	3.36	118.73	111.50
3	G	304	DGA	OG1-CA1-CA2	3.34	122.40	111.91
3	A	303[B]	DGA	OG2-CB1-CB2	3.23	118.46	111.50
3	A	304	DGA	CG2-OG2-CB1	-3.10	110.17	117.79
3	G	303	DGA	CG1-CG2-CG3	-2.94	104.93	111.80
3	V	303	DGA	OG1-CA1-CA2	2.84	120.83	111.91
3	V	303	DGA	OG1-CA1-OA1	-2.81	116.51	123.59
3	G	304	DGA	OG2-CB1-OB1	-2.79	116.95	123.70
3	P	303	DGA	OG1-CA1-CA2	2.79	120.66	111.91
3	A	303[B]	DGA	CG2-OG2-CB1	-2.76	110.99	117.79
3	D	303	DGA	OG1-CA1-CA2	2.75	120.54	111.91
3	A	304	DGA	OG1-CA1-CA2	2.68	120.32	111.91
3	P	303	DGA	CG1-CG2-CG3	-2.66	105.58	111.80
3	A	303[A]	DGA	OG1-CA1-CA2	2.57	119.99	111.91
3	M	303	DGA	CA3-CA2-CA1	-2.53	104.43	113.62
3	S	303	DGA	OG1-CG1-CG2	2.52	115.77	108.43
3	M	303	DGA	CB3-CB2-CB1	-2.51	104.48	113.62
3	J	303	DGA	OG2-CB1-CB2	2.49	116.86	111.50
3	A	303[B]	DGA	OG1-CA1-CA2	2.44	119.56	111.91
3	V	303	DGA	OG2-CB1-OB1	-2.44	117.81	123.70
3	P	303	DGA	OG1-CA1-OA1	-2.44	117.44	123.59
5	J	304	DPV	C4-C5-N	-2.38	107.83	115.78
3	A	304	DGA	OG2-CB1-OB1	-2.37	117.97	123.70
3	A	303[A]	DGA	CG2-OG2-CB1	-2.33	112.06	117.79
3	G	303	DGA	OG1-CA1-CA2	2.29	119.11	111.91
3	D	303	DGA	OG1-CA1-OA1	-2.29	117.82	123.59
3	A	303[A]	DGA	OG2-CB1-OB1	-2.24	118.30	123.70
3	D	303	DGA	OG2-CB1-CB2	2.22	116.30	111.50
3	J	303	DGA	OG1-CA1-CA2	2.22	118.86	111.91
3	S	303	DGA	OG1-CA1-OA1	-2.21	118.00	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	303	DGA	CB6-CB5-CB4	-2.20	103.25	114.42
3	J	303	DGA	OG1-CA1-OA1	-2.17	118.12	123.59
3	M	303	DGA	OG1-CA1-CA2	2.15	118.66	111.91
3	G	303	DGA	CG2-OG2-CB1	-2.11	112.60	117.79
3	G	304	DGA	OG1-CA1-OA1	-2.10	118.29	123.59
3	P	303	DGA	OG2-CB1-OB1	-2.09	118.65	123.70
3	D	303	DGA	OG2-CB1-OB1	-2.09	118.65	123.70
3	G	303	DGA	OG2-CB1-OB1	-2.06	118.72	123.70

There are no chirality outliers.

All (197) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303[B]	DGA	OB1-CB1-OG2-CG2
3	A	304	DGA	CA2-CA1-OG1-CG1
3	A	304	DGA	OA1-CA1-OG1-CG1
3	A	304	DGA	CG1-CG2-CG3-OXT
3	A	304	DGA	OG2-CG2-CG3-OXT
3	G	304	DGA	CB2-CB1-OG2-CG2
3	G	304	DGA	OB1-CB1-OG2-CG2
3	P	303	DGA	CB2-CB1-OG2-CG2
3	P	303	DGA	CG1-CG2-CG3-OXT
3	P	303	DGA	OG2-CG2-CG3-OXT
3	S	303	DGA	CB2-CB1-OG2-CG2
5	D	304	DPV	C4-O4P-P-O3P
5	D	304	DPV	O4P-C4-C5-N
5	J	304	DPV	C1-O3P-P-O2P
5	J	304	DPV	C4-O4P-P-O3P
5	M	304[A]	DPV	C1-O3P-P-O2P
5	M	304[A]	DPV	O4P-C4-C5-N
5	M	304[B]	DPV	C1-O3P-P-O2P
5	M	304[B]	DPV	C4-O4P-P-O2P
5	P	304	DPV	C1-O3P-P-O1P
5	P	304	DPV	C1-O3P-P-O2P
5	P	304	DPV	C1-O3P-P-O4P
5	P	304	DPV	C4-O4P-P-O2P
5	P	304	DPV	C4-O4P-P-O3P
5	P	304	DPV	O4P-C4-C5-N
5	S	304	DPV	C1-O3P-P-O1P
5	S	304	DPV	C1-O3P-P-O2P
5	S	304	DPV	C1-O3P-P-O4P
5	S	304	DPV	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
5	S	304	DPV	C4-O4P-P-O2P
5	S	304	DPV	C4-O4P-P-O3P
5	V	304	DPV	C4-O4P-P-O2P
5	V	304	DPV	C4-O4P-P-O3P
5	V	304	DPV	O4P-C4-C5-N
3	G	304	DGA	OA1-CA1-OG1-CG1
3	P	303	DGA	OB1-CB1-OG2-CG2
3	S	303	DGA	OB1-CB1-OG2-CG2
3	S	303	DGA	OA1-CA1-OG1-CG1
3	G	304	DGA	CA2-CA1-OG1-CG1
3	P	303	DGA	CA2-CA1-OG1-CG1
3	A	303[B]	DGA	CB2-CB1-OG2-CG2
3	G	303	DGA	CA2-CA1-OG1-CG1
3	S	303	DGA	CA2-CA1-OG1-CG1
3	G	303	DGA	OA1-CA1-OG1-CG1
3	P	303	DGA	OA1-CA1-OG1-CG1
3	V	303	DGA	CB1-CB2-CB3-CB4
3	A	304	DGA	CB1-CB2-CB3-CB4
3	A	303[A]	DGA	CA2-CA1-OG1-CG1
3	A	304	DGA	CA2-CA3-CA4-CA5
3	A	303[B]	DGA	CA2-CA1-OG1-CG1
5	M	304[B]	DPV	O3P-C1-C2-C3
3	A	303[A]	DGA	CA1-CA2-CA3-CA4
3	G	304	DGA	CB1-CB2-CB3-CB4
3	A	304	DGA	CB2-CB1-OG2-CG2
3	A	303[B]	DGA	OA1-CA1-OG1-CG1
3	A	303[B]	DGA	CA3-CA4-CA5-CA6
3	A	303[A]	DGA	OA1-CA1-OG1-CG1
3	G	304	DGA	CB2-CB3-CB4-CB5
5	J	304	DPV	C1-O3P-P-O4P
5	M	304[A]	DPV	C4-O4P-P-O3P
3	A	304	DGA	OB1-CB1-OG2-CG2
3	G	303	DGA	CB2-CB1-OG2-CG2
3	D	303	DGA	CB3-CB4-CB5-CB6
5	M	304[A]	DPV	C16-C15-C3-C2
5	M	304[B]	DPV	C17-C18-C19-C20
5	M	304[B]	DPV	C18-C19-C20-C21
3	A	303[A]	DGA	CA4-CA5-CA6-CA7
3	J	303	DGA	CA3-CA4-CA5-CA6
3	G	303	DGA	OB1-CB1-OG2-CG2
5	J	304	DPV	C15-C16-C17-C18
5	V	304	DPV	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
5	D	304	DPV	C19-C20-C21-C22
3	G	303	DGA	CB2-CB3-CB4-CB5
5	S	304	DPV	C16-C15-C3-C2
5	S	304	DPV	C15-C16-C17-C18
5	M	304[A]	DPV	C18-C19-C20-C21
5	M	304[A]	DPV	C19-C20-C21-C22
5	J	304	DPV	C17-C18-C19-C20
3	A	303[B]	DGA	CA1-CA2-CA3-CA4
3	V	303	DGA	CA4-CA5-CA6-CA7
5	S	304	DPV	C17-C18-C19-C20
5	V	304	DPV	C19-C20-C21-C22
3	M	303	DGA	CB2-CB3-CB4-CB5
5	S	304	DPV	C3-C15-C16-C17
3	D	303	DGA	CA4-CA5-CA6-CA7
5	J	304	DPV	C1-C2-C3-C15
3	J	303	DGA	CB2-CB3-CB4-CB5
3	J	303	DGA	CA2-CA3-CA4-CA5
3	P	303	DGA	CB4-CB5-CB6-CB7
3	S	303	DGA	CB3-CB4-CB5-CB6
5	V	304	DPV	C16-C15-C3-C2
5	P	304	DPV	C1-C2-C3-C15
3	G	304	DGA	CB3-CB4-CB5-CB6
5	D	304	DPV	C18-C19-C20-C21
3	A	304	DGA	CB4-CB5-CB6-CB7
5	D	304	DPV	C15-C16-C17-C18
5	M	304[B]	DPV	C1-C2-C3-C15
5	M	304[A]	DPV	C16-C17-C18-C19
5	V	304	DPV	C16-C17-C18-C19
3	D	303	DGA	CA3-CA4-CA5-CA6
5	M	304[B]	DPV	C1-O3P-P-O4P
5	M	304[B]	DPV	C4-O4P-P-O3P
3	A	304	DGA	CA1-CA2-CA3-CA4
3	M	303	DGA	CA2-CA3-CA4-CA5
5	V	304	DPV	C18-C19-C20-C21
5	V	304	DPV	C2-C1-O3P-P
5	D	304	DPV	C20-C21-C22-C23
3	S	303	DGA	CB4-CB5-CB6-CB7
5	V	304	DPV	C15-C16-C17-C18
3	A	304	DGA	CA3-CA4-CA5-CA6
3	A	303[A]	DGA	OG1-CG1-CG2-CG3
3	G	304	DGA	OG1-CG1-CG2-CG3
3	A	304	DGA	CB2-CB3-CB4-CB5

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Mol	Chain	Res	Type	Atoms
3	V	303	DGA	CB2-CB3-CB4-CB5
5	D	304	DPV	O3P-C1-C2-C3
5	S	304	DPV	O3P-C1-C2-C3
3	S	303	DGA	CB5-CB6-CB7-CB8
3	V	303	DGA	CB3-CB4-CB5-CB6
5	M	304[A]	DPV	C20-C21-C22-C23
3	A	303[A]	DGA	OG1-CG1-CG2-OG2
3	A	304	DGA	CA5-CA6-CA7-CA8
5	J	304	DPV	C16-C17-C18-C19
5	M	304[A]	DPV	C3-C15-C16-C17
3	G	304	DGA	CA2-CA3-CA4-CA5
3	P	303	DGA	CA5-CA6-CA7-CA8
5	M	304[B]	DPV	C3-C15-C16-C17
5	J	304	DPV	C20-C21-C22-C23
3	A	303[A]	DGA	CB2-CB3-CB4-CB5
3	S	303	DGA	CA2-CA3-CA4-CA5
3	M	303	DGA	CA5-CA6-CA7-CA8
3	M	303	DGA	CA1-CA2-CA3-CA4
3	G	303	DGA	CB4-CB5-CB6-CB7
5	M	304[A]	DPV	C1-O3P-P-O4P
3	A	304	DGA	OG1-CG1-CG2-OG2
5	P	304	DPV	O3P-C1-C2-C3
5	D	304	DPV	C16-C15-C3-C2
3	M	303	DGA	CB5-CB6-CB7-CB8
3	A	303[A]	DGA	CB1-CB2-CB3-CB4
3	S	303	DGA	CA5-CA6-CA7-CA8
3	J	303	DGA	CB3-CB4-CB5-CB6
3	V	303	DGA	CB5-CB6-CB7-CB8
5	M	304[B]	DPV	C16-C15-C3-C2
5	J	304	DPV	C3-C15-C16-C17
3	S	303	DGA	CA3-CA4-CA5-CA6
3	G	304	DGA	CB5-CB6-CB7-CB8
5	M	304[A]	DPV	O3P-C1-C2-C3
5	D	304	DPV	C1-O3P-P-O1P
5	D	304	DPV	C4-O4P-P-O1P
5	J	304	DPV	C1-O3P-P-O1P
5	J	304	DPV	C4-O4P-P-O1P
5	M	304[A]	DPV	C1-O3P-P-O1P
5	M	304[A]	DPV	C4-O4P-P-O1P
5	M	304[B]	DPV	C4-O4P-P-O1P
5	P	304	DPV	C4-O4P-P-O1P
5	P	304	DPV	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
3	J	303	DGA	CA2-CA1-OG1-CG1
5	J	304	DPV	O4P-C4-C5-N
5	S	304	DPV	O4P-C4-C5-N
3	G	304	DGA	OG1-CG1-CG2-OG2
5	D	304	DPV	C3-C15-C16-C17
3	V	303	DGA	CB4-CB5-CB6-CB7
3	G	303	DGA	CG1-CG2-OG2-CB1
5	P	304	DPV	C18-C19-C20-C21
5	M	304[A]	DPV	C17-C18-C19-C20
3	A	303[B]	DGA	OG1-CG1-CG2-OG2
3	A	303[B]	DGA	OG1-CG1-CG2-CG3
3	J	303	DGA	OA1-CA1-OG1-CG1
3	M	303	DGA	CB4-CB5-CB6-CB7
5	S	304	DPV	C19-C20-C21-C22
3	P	303	DGA	CG1-CG2-OG2-CB1
3	A	303[B]	DGA	CA4-CA5-CA6-CA7
5	M	304[B]	DPV	C19-C20-C21-C22
3	J	303	DGA	CA4-CA5-CA6-CA7
3	V	303	DGA	CA2-CA3-CA4-CA5
3	G	304	DGA	CA1-CA2-CA3-CA4
3	M	303	DGA	OA1-CA1-OG1-CG1
3	A	303[B]	DGA	OG2-CG2-CG3-OXT
3	M	303	DGA	CA2-CA1-OG1-CG1
3	A	303[A]	DGA	OG2-CB1-CB2-CB3
3	D	303	DGA	OG1-CA1-CA2-CA3
3	P	303	DGA	OG1-CA1-CA2-CA3
3	A	304	DGA	OG1-CG1-CG2-CG3
3	V	303	DGA	OG1-CA1-CA2-CA3
3	D	303	DGA	OG2-CB1-CB2-CB3
3	A	303[A]	DGA	OB1-CB1-CB2-CB3
5	M	304[B]	DPV	C20-C21-C22-C23
3	M	303	DGA	OB1-CB1-OG2-CG2
3	V	303	DGA	OA1-CA1-CA2-CA3
3	M	303	DGA	CA3-CA4-CA5-CA6
3	D	303	DGA	OA1-CA1-CA2-CA3
3	D	303	DGA	CB2-CB3-CB4-CB5
3	P	303	DGA	OA1-CA1-CA2-CA3
3	G	303	DGA	OG1-CA1-CA2-CA3
3	G	304	DGA	CA4-CA5-CA6-CA7
3	G	304	DGA	OG2-CB1-CB2-CB3
3	D	303	DGA	OB1-CB1-CB2-CB3
3	G	303	DGA	OA1-CA1-CA2-CA3

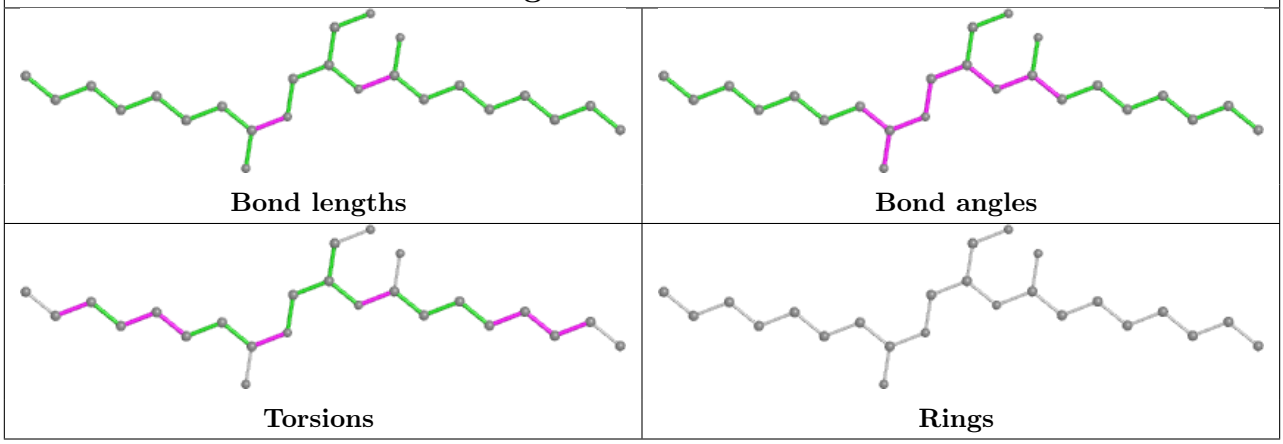
There are no ring outliers.

17 monomers are involved in 41 short contacts:

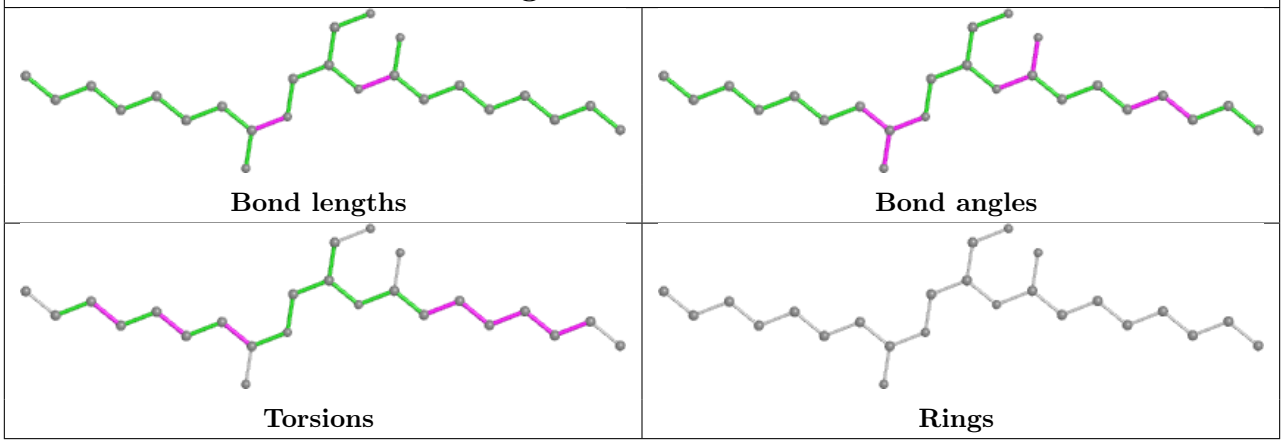
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	304[B]	DPV	1	0
4	S	305	EOH	1	0
3	G	303	DGA	4	0
4	A	305	EOH	3	0
3	A	303[A]	DGA	1	0
3	P	303	DGA	5	0
5	J	304	DPV	1	0
5	P	304	DPV	2	0
3	J	303	DGA	2	0
5	S	304	DPV	2	0
3	M	303	DGA	5	0
3	D	303	DGA	1	0
5	M	304[A]	DPV	6	0
3	G	304	DGA	3	0
3	A	303[B]	DGA	1	0
5	V	304	DPV	3	0
5	D	304	DPV	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 then 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.

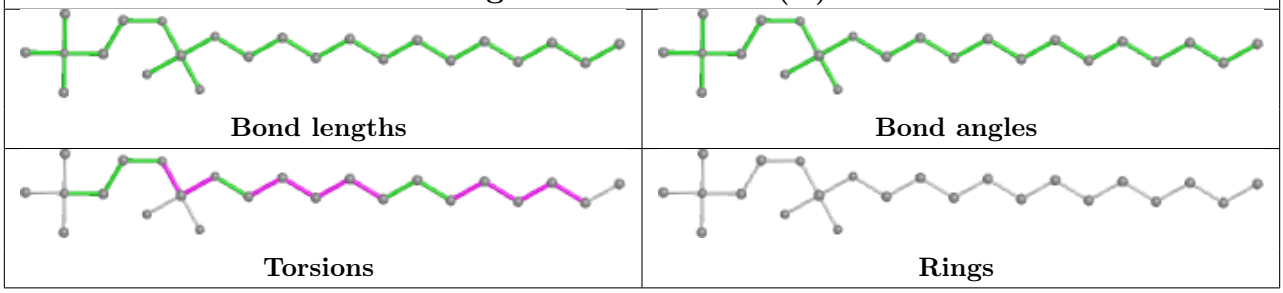
Ligand DGA S 303



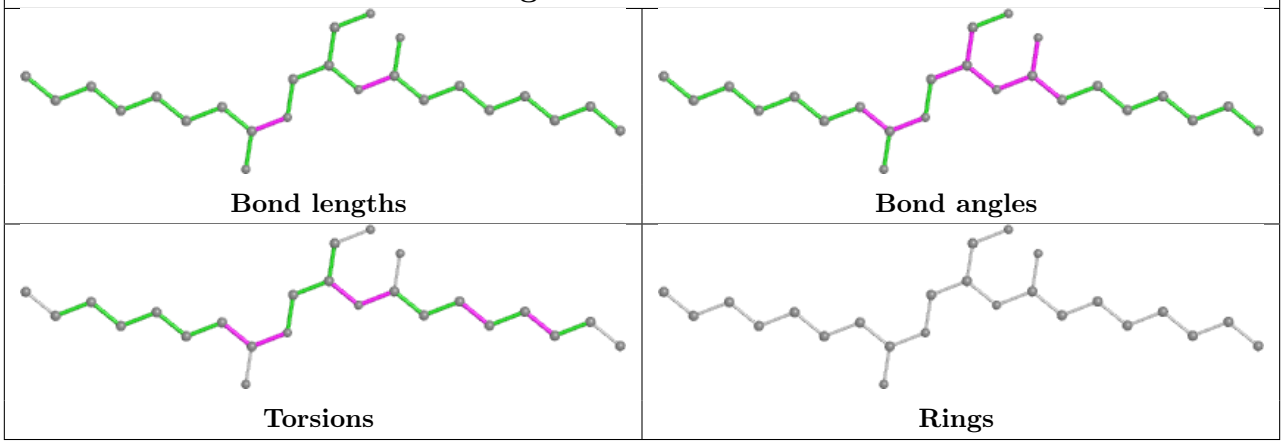
Ligand DGA V 303



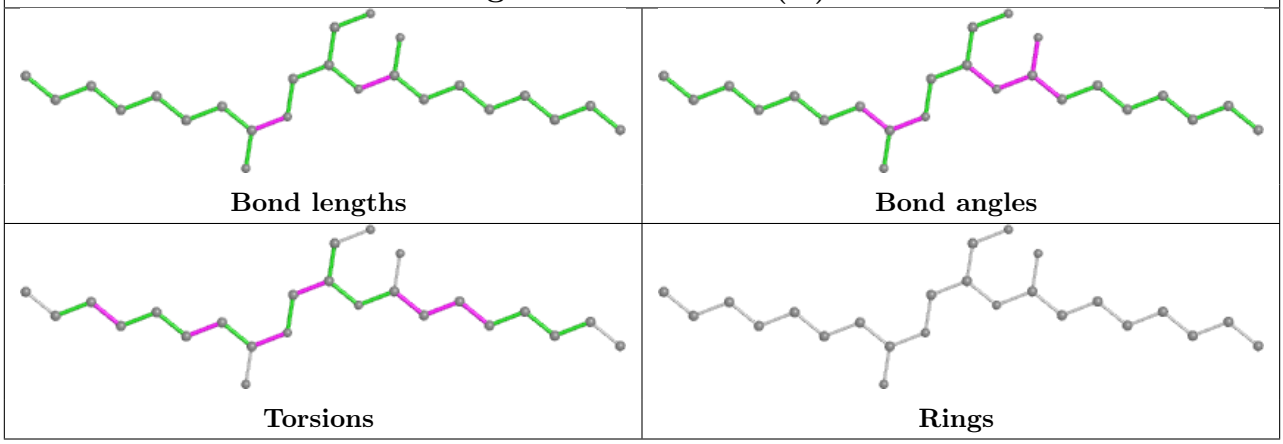
Ligand DPV M 304 (B)



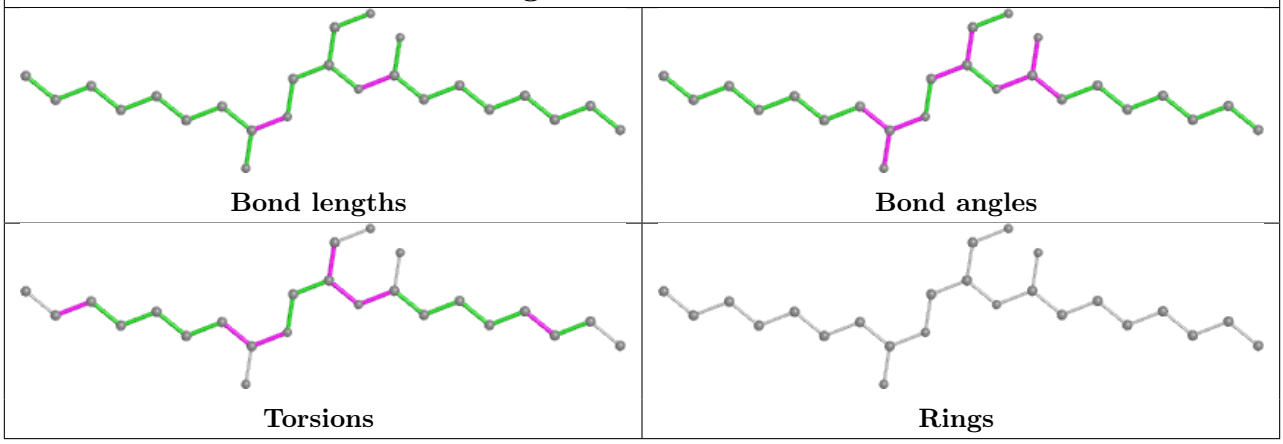
Ligand DGA G 303



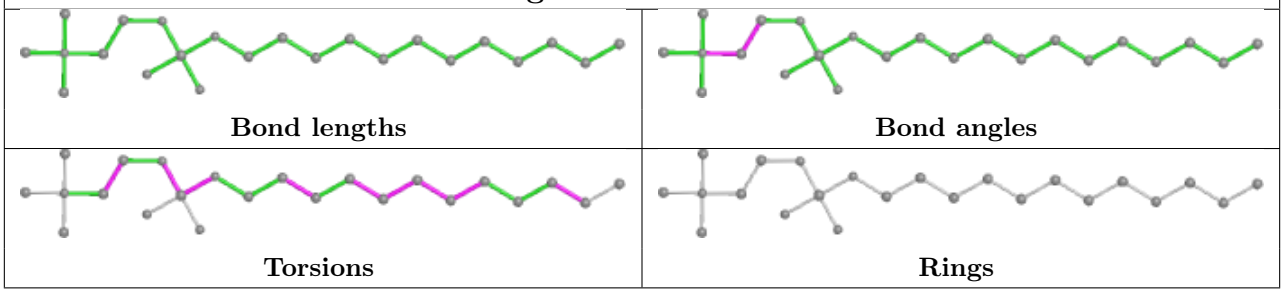
Ligand DGA A 303 (A)



Ligand DGA P 303



Ligand DPV J 304



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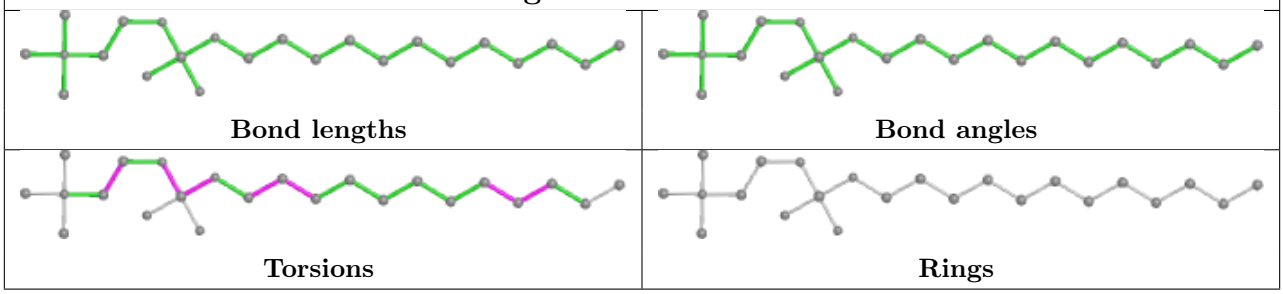
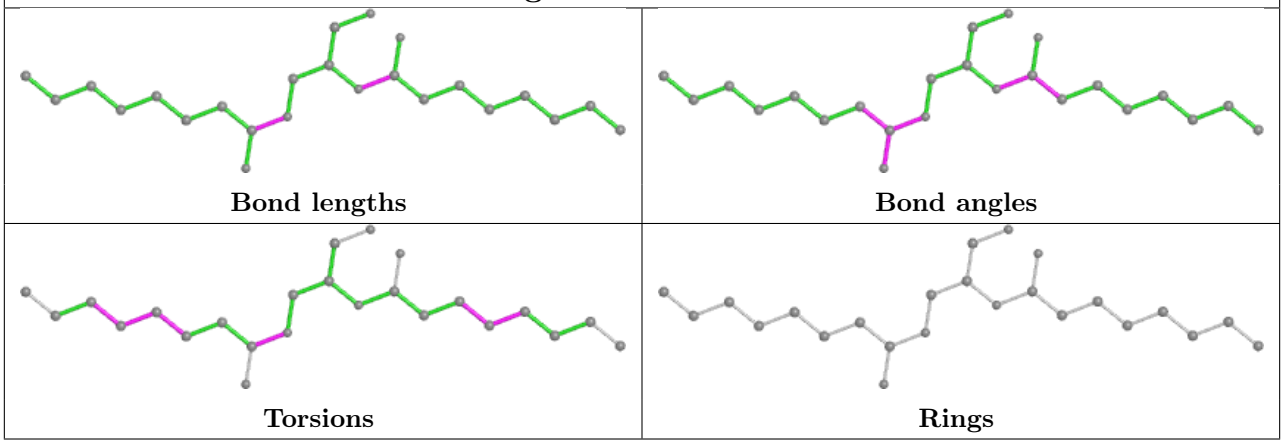
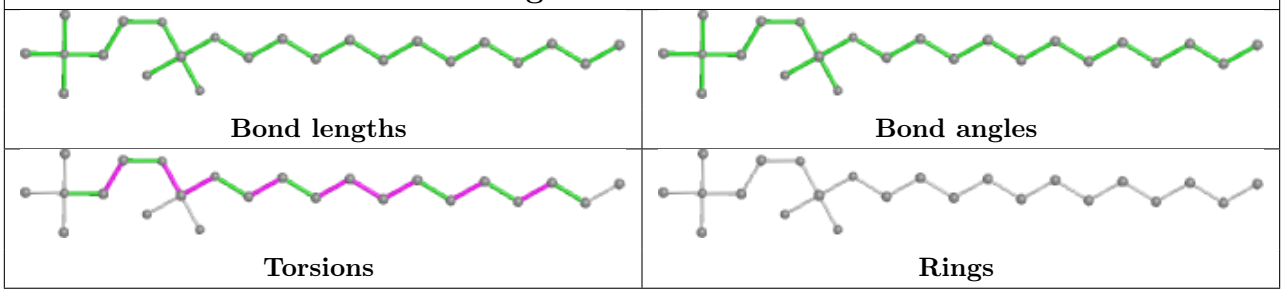


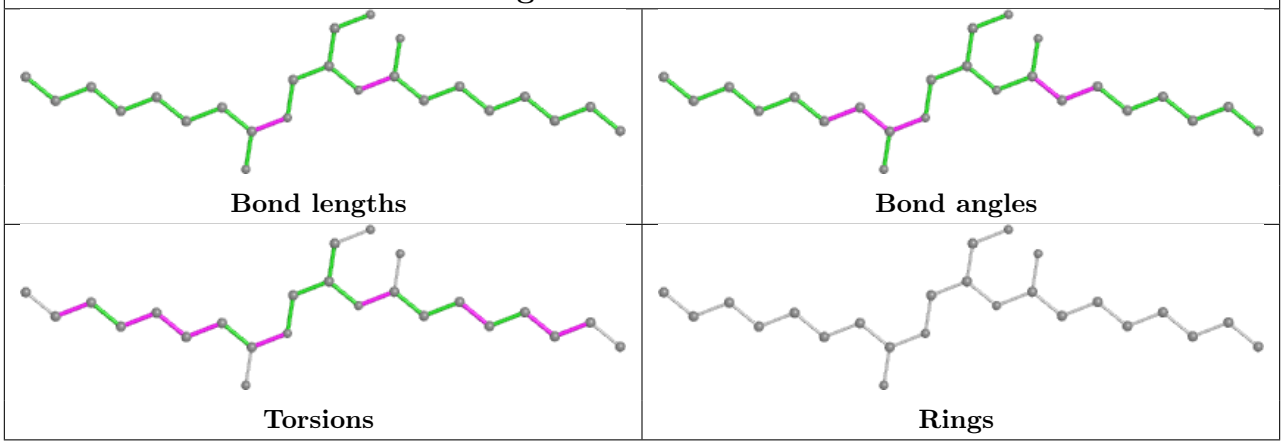
Ligand DGA J 303



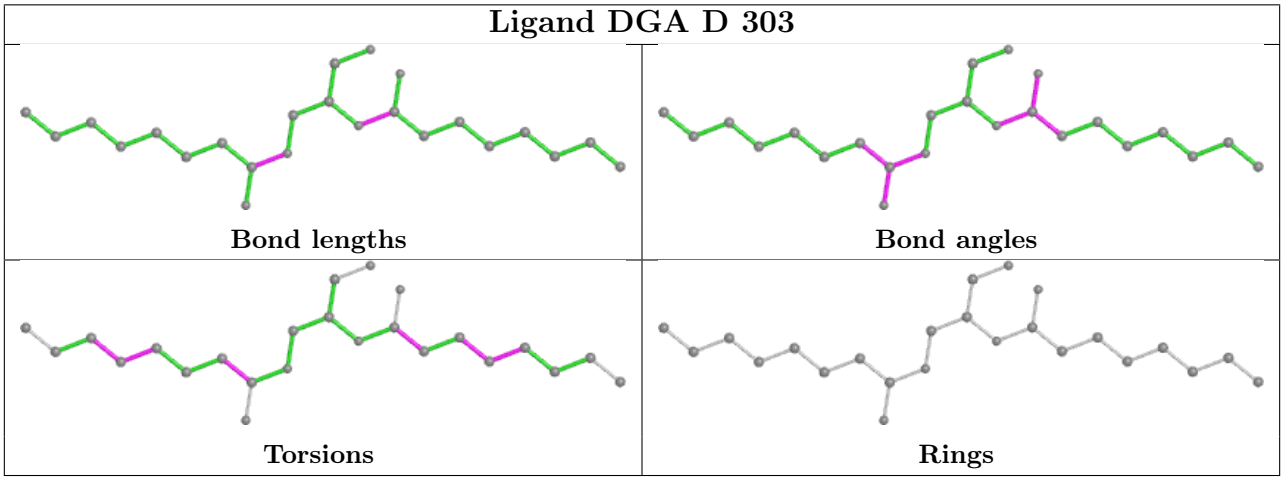
Ligand DPV S 304



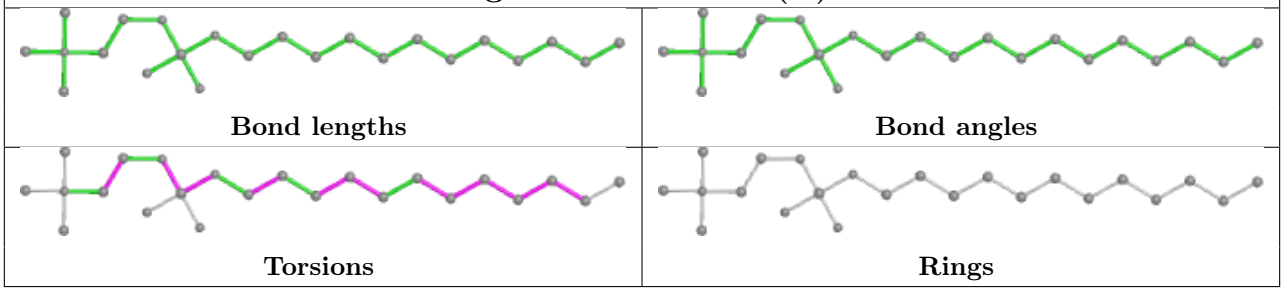
Ligand DGA M 303



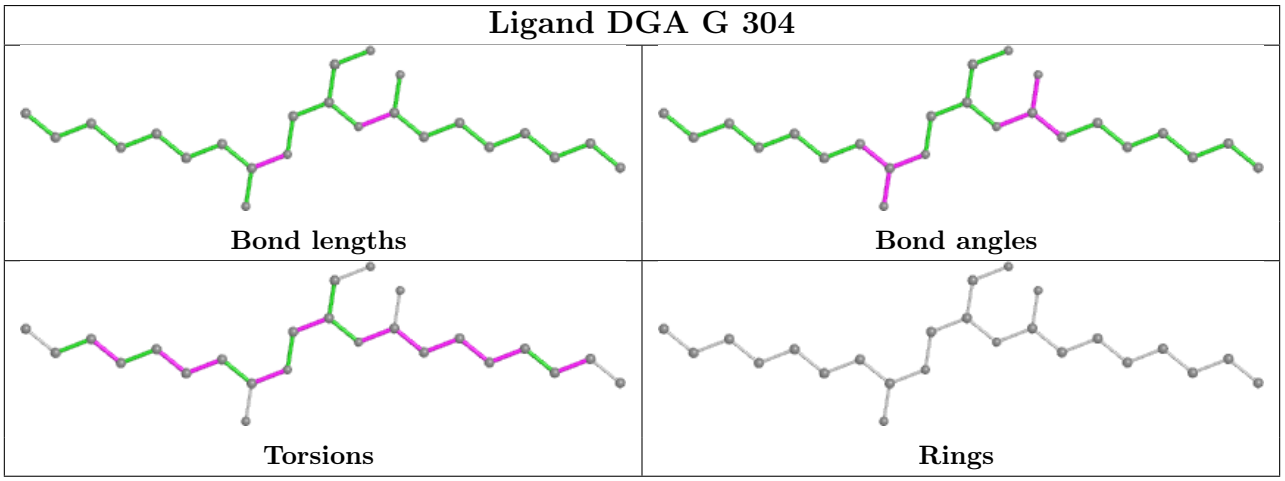
Ligand DGA D 303



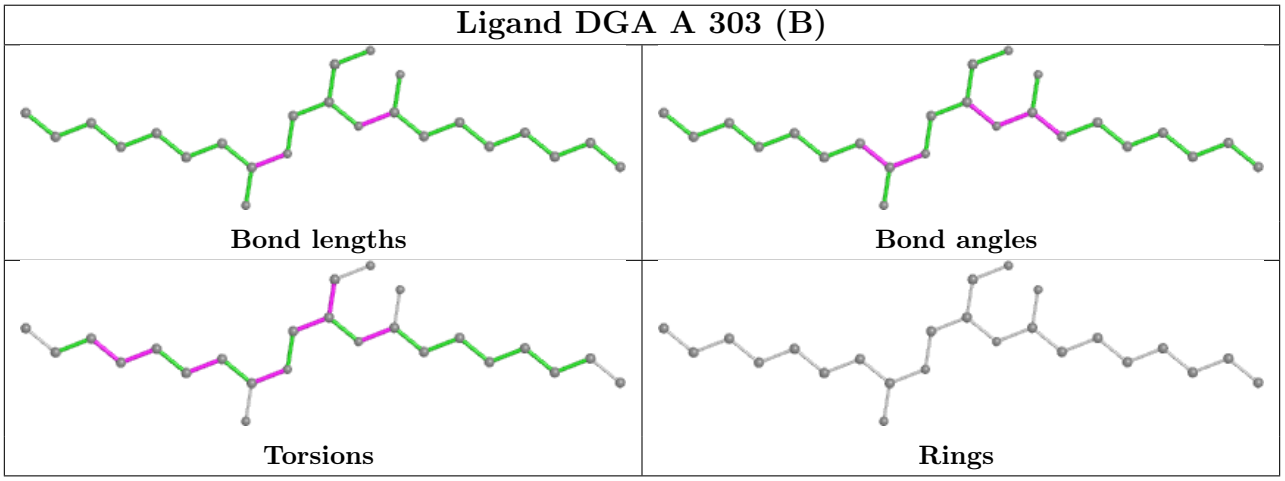
Ligand DPV M 304 (A)



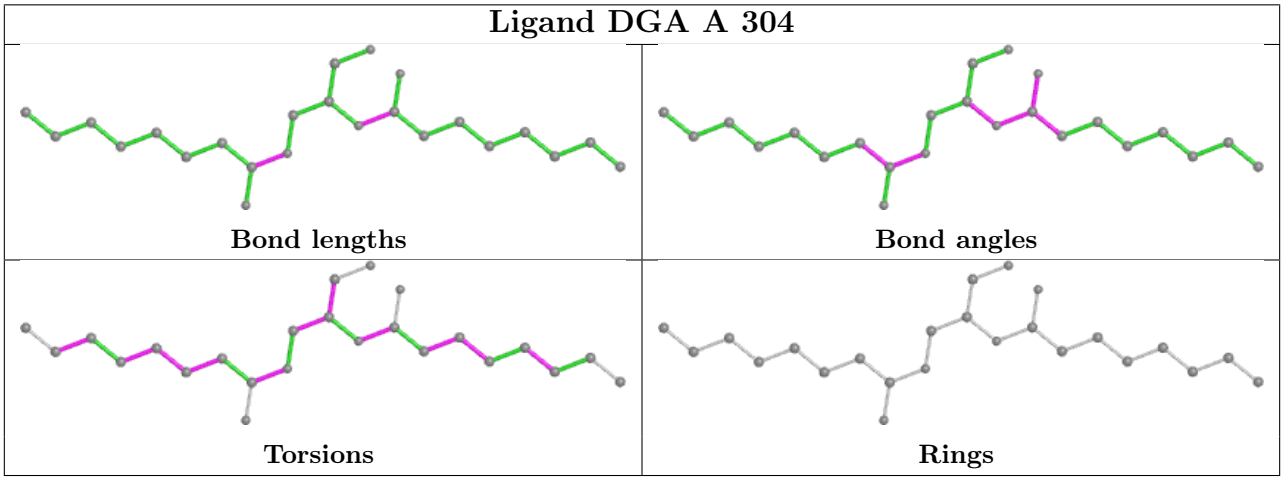
Ligand DGA G 304

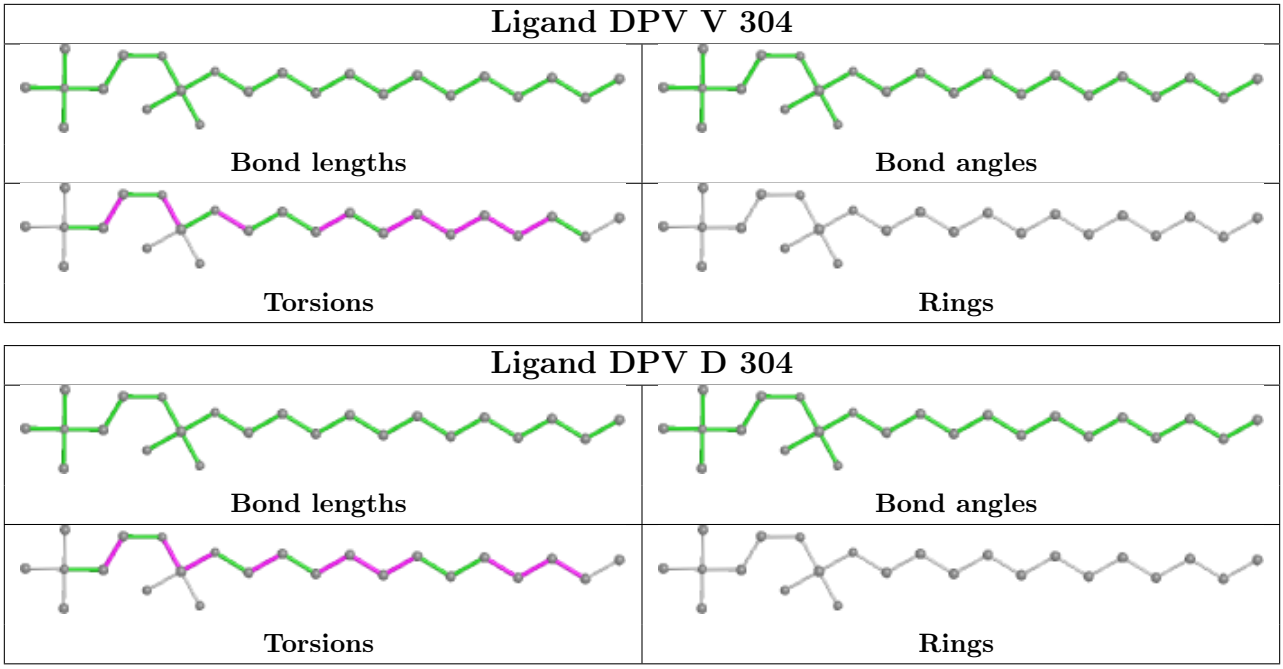


Ligand DGA A 303 (B)



Ligand DGA A 304





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, 95^{th} 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	52/53 (98%)	-0.27	0 100 100	25, 39, 57, 67	0
1	D	51/53 (96%)	-0.23	2 (3%) 39 45	19, 32, 64, 78	0
1	G	52/53 (98%)	-0.12	1 (1%) 66 74	26, 40, 56, 64	0
1	J	51/53 (96%)	-0.21	2 (3%) 39 45	20, 32, 62, 72	0
1	M	52/53 (98%)	-0.29	1 (1%) 66 74	19, 33, 64, 73	0
1	P	52/53 (98%)	-0.18	0 100 100	26, 40, 56, 62	0
1	S	52/53 (98%)	-0.19	0 100 100	27, 40, 57, 63	0
1	V	52/53 (98%)	-0.33	0 100 100	19, 32, 63, 68	0
All	All	414/424 (97%)	-0.23	6 (1%) 75 82	19, 36, 62, 78	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	277	ALA	4.3
1	J	279	LEU	3.3
1	D	279	LEU	2.8
1	M	279	LEU	2.7
1	D	277	ALA	2.6
1	G	278	ASN	2.3

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

There are no monosaccharides in this entry.

6.4 Ligands (i)

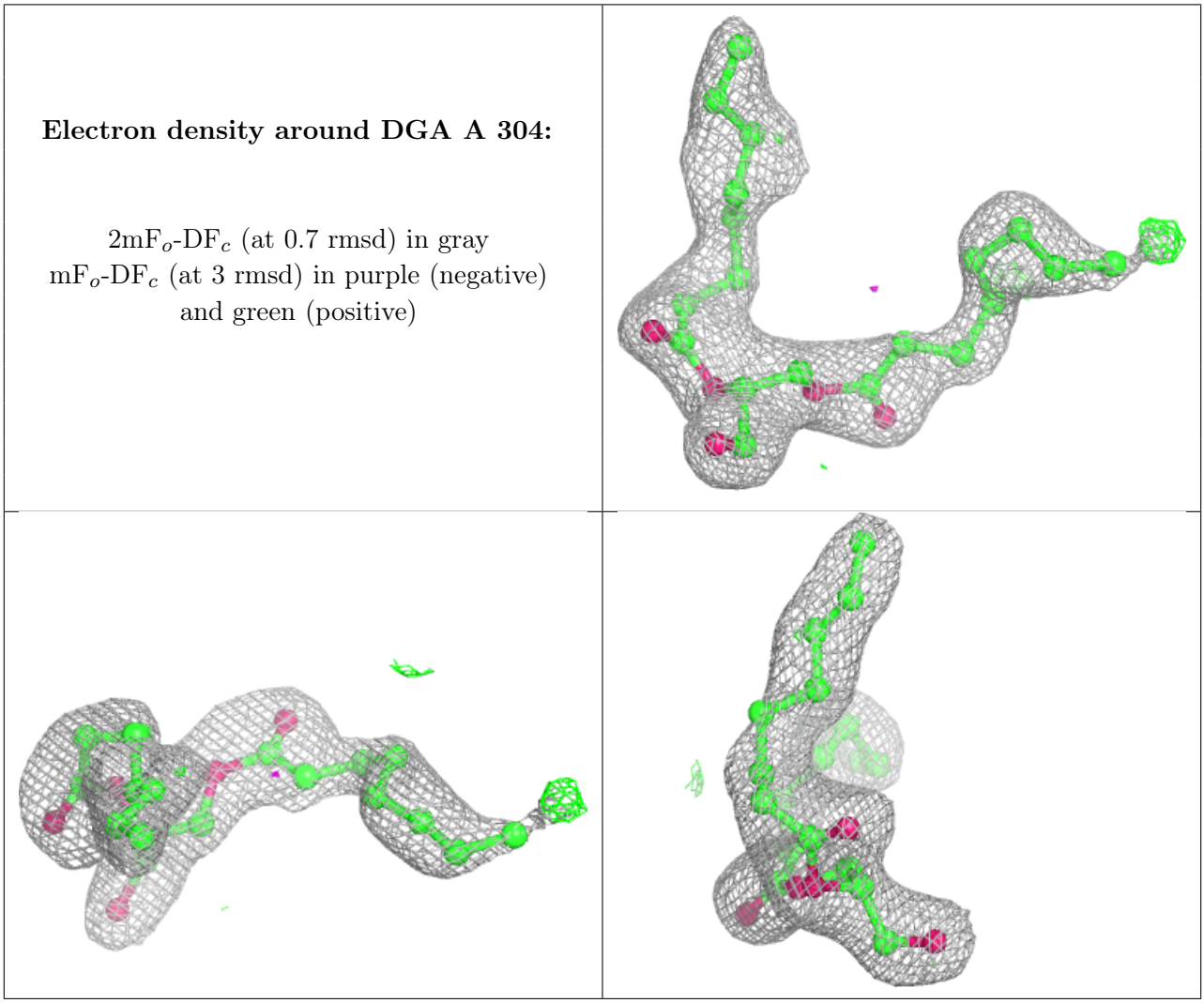
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	DGA	A	304	24/44	0.88	0.11	56,74,85,86	0
3	DGA	G	304	24/44	0.90	0.11	55,68,77,80	0
3	DGA	S	303	24/44	0.91	0.10	42,57,75,76	0
3	DGA	A	303[B]	24/44	0.92	0.11	44,55,60,63	24
3	DGA	P	303	24/44	0.92	0.10	49,62,68,71	0
3	DGA	A	303[A]	24/44	0.92	0.11	44,54,62,64	24
4	EOH	S	305	3/3	0.92	0.12	52,52,55,60	0
5	DPV	P	304	23/23	0.92	0.18	65,78,94,99	0
3	DGA	G	303	24/44	0.94	0.08	42,60,65,67	0
5	DPV	S	304	23/23	0.94	0.12	53,68,76,78	0
2	ZN	V	301	1/1	0.95	0.04	38,38,38,38	0
2	ZN	M	301	1/1	0.95	0.05	37,37,37,37	0
4	EOH	A	305	3/3	0.95	0.09	32,32,40,46	0
5	DPV	M	304[A]	23/23	0.96	0.13	24,39,49,55	23
5	DPV	M	304[B]	23/23	0.96	0.13	32,38,56,58	23
2	ZN	D	301	1/1	0.96	0.05	37,37,37,37	0
5	DPV	D	304	23/23	0.96	0.10	33,50,62,64	0
5	DPV	V	304	23/23	0.96	0.09	32,45,55,56	0
5	DPV	J	304	23/23	0.97	0.09	31,46,61,63	0
3	DGA	V	303	24/44	0.97	0.09	18,32,64,73	0
3	DGA	J	303	24/44	0.97	0.07	18,35,60,65	0
2	ZN	P	302	1/1	0.98	0.05	33,33,33,33	0
3	DGA	M	303	24/44	0.98	0.08	18,32,62,64	0
2	ZN	S	301	1/1	0.98	0.06	32,32,32,32	0
2	ZN	S	302	1/1	0.98	0.05	32,32,32,32	0
3	DGA	D	303	24/44	0.98	0.08	17,30,62,68	0
2	ZN	J	301	1/1	0.98	0.05	37,37,37,37	0
2	ZN	V	302	1/1	0.98	0.05	30,30,30,30	0
2	ZN	G	301	1/1	0.99	0.06	31,31,31,31	0
2	ZN	G	302	1/1	0.99	0.04	32,32,32,32	0
2	ZN	A	302	1/1	0.99	0.05	32,32,32,32	0
2	ZN	J	302	1/1	0.99	0.07	29,29,29,29	0
2	ZN	A	301	1/1	0.99	0.05	30,30,30,30	0
2	ZN	M	302	1/1	0.99	0.05	30,30,30,30	0
2	ZN	P	301	1/1	0.99	0.05	31,31,31,31	0
2	ZN	D	302	1/1	0.99	0.06	29,29,29,29	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.

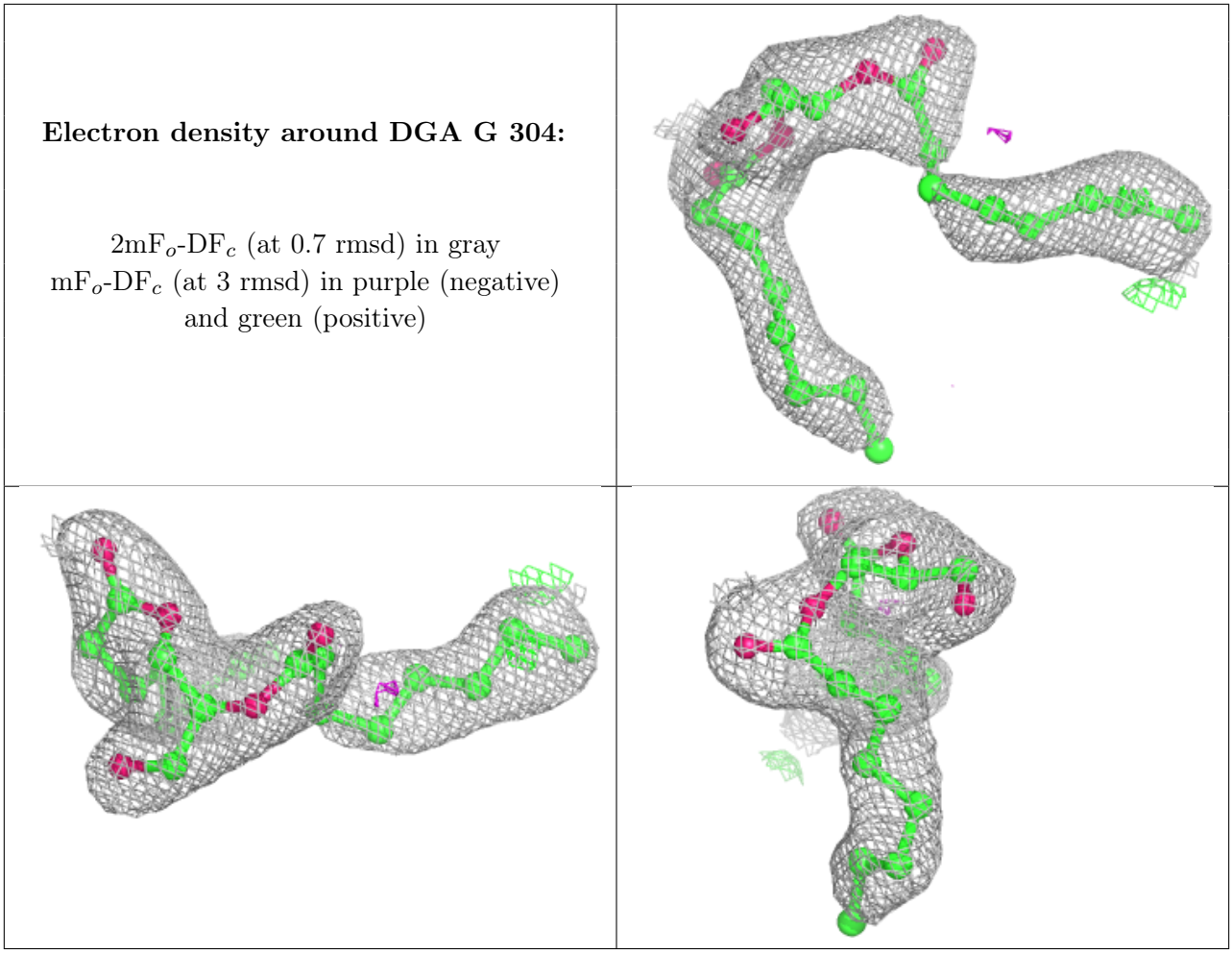
Electron density around DGA A 304:

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



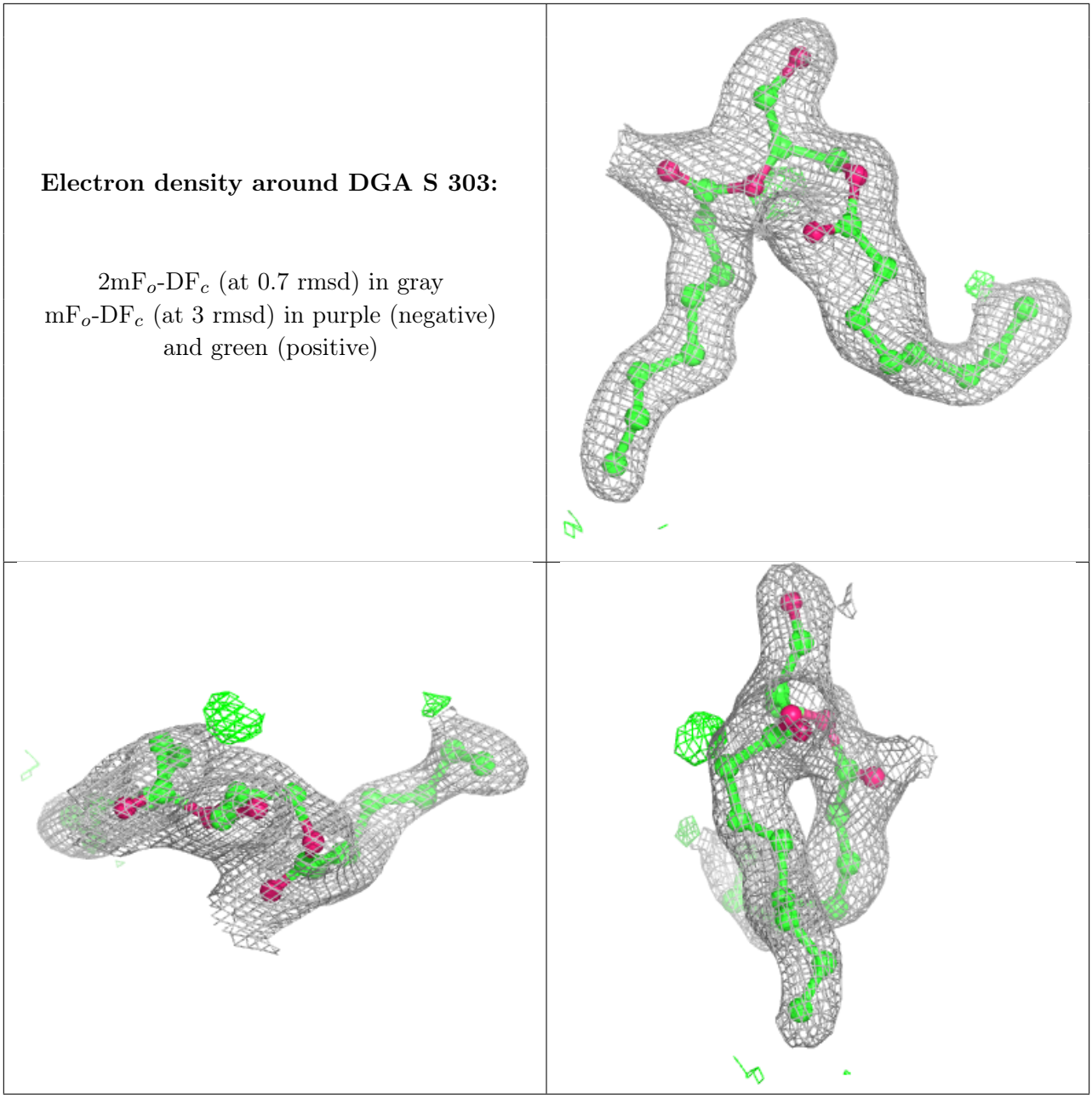
Electron density around DGA G 304:

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



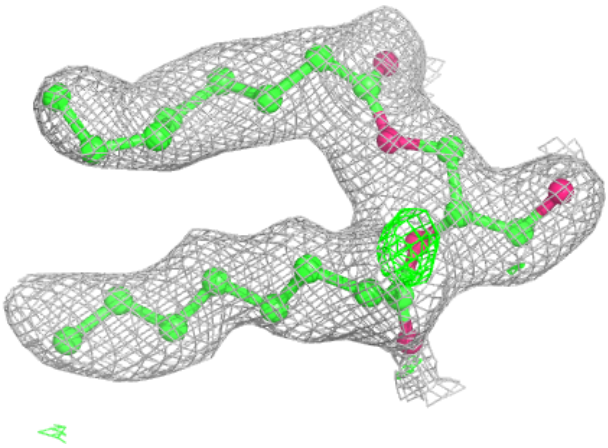
Electron density around DGA S 303:

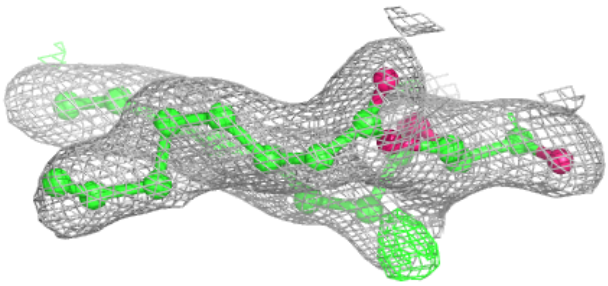
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

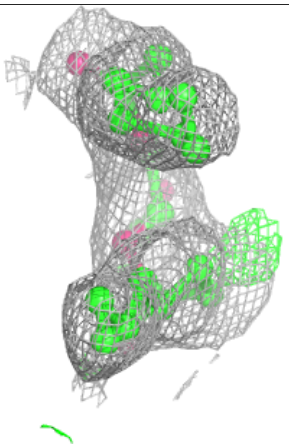


Electron density around DGA A 303 (B):

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

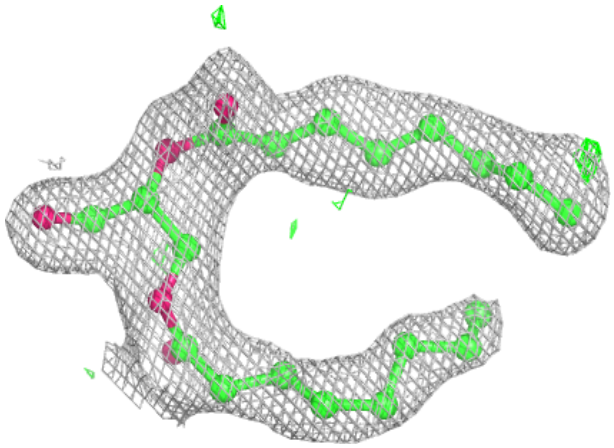


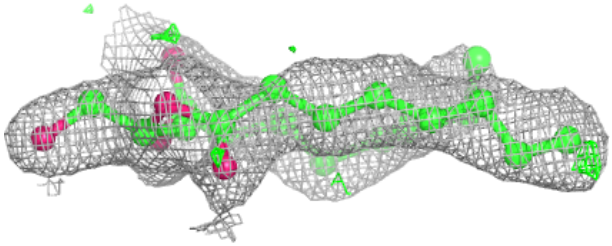


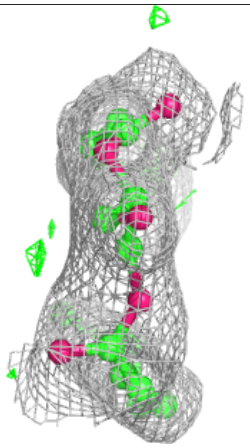


Electron density around DGA P 303:

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

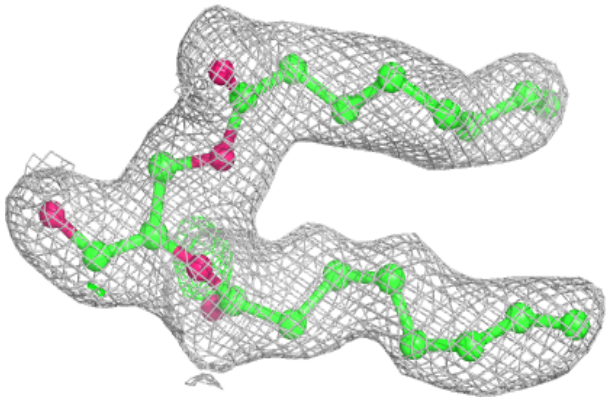


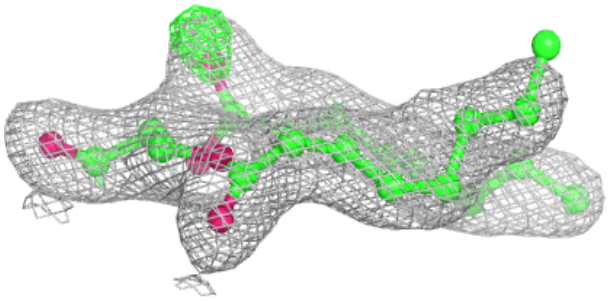


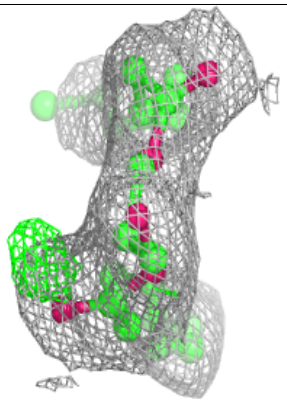


Electron density around DGA A 303 (A):

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

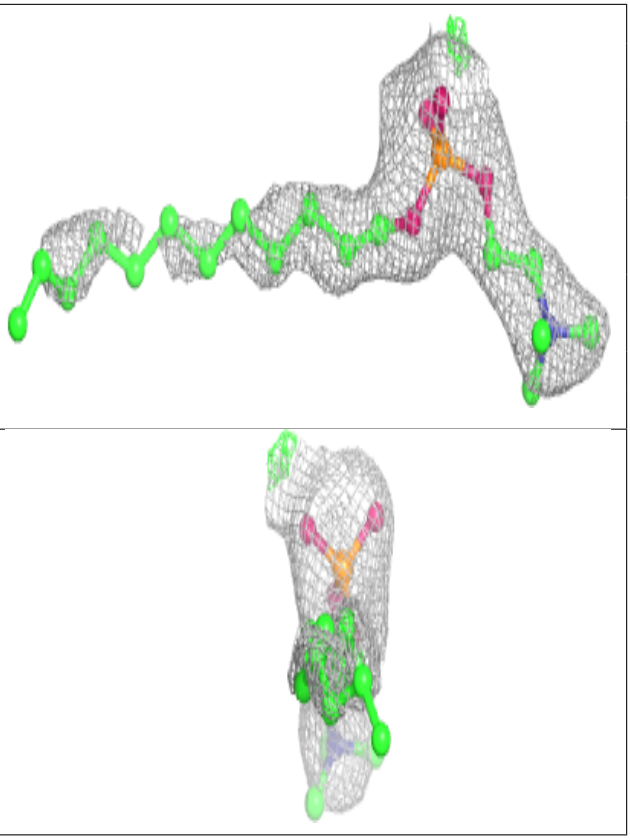


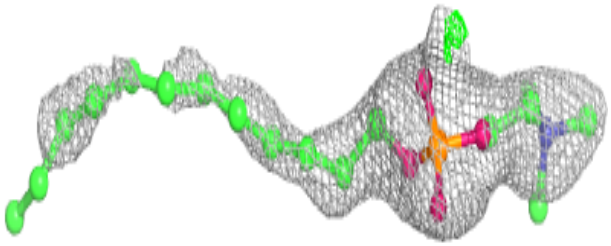




Electron density around DPV P 304:

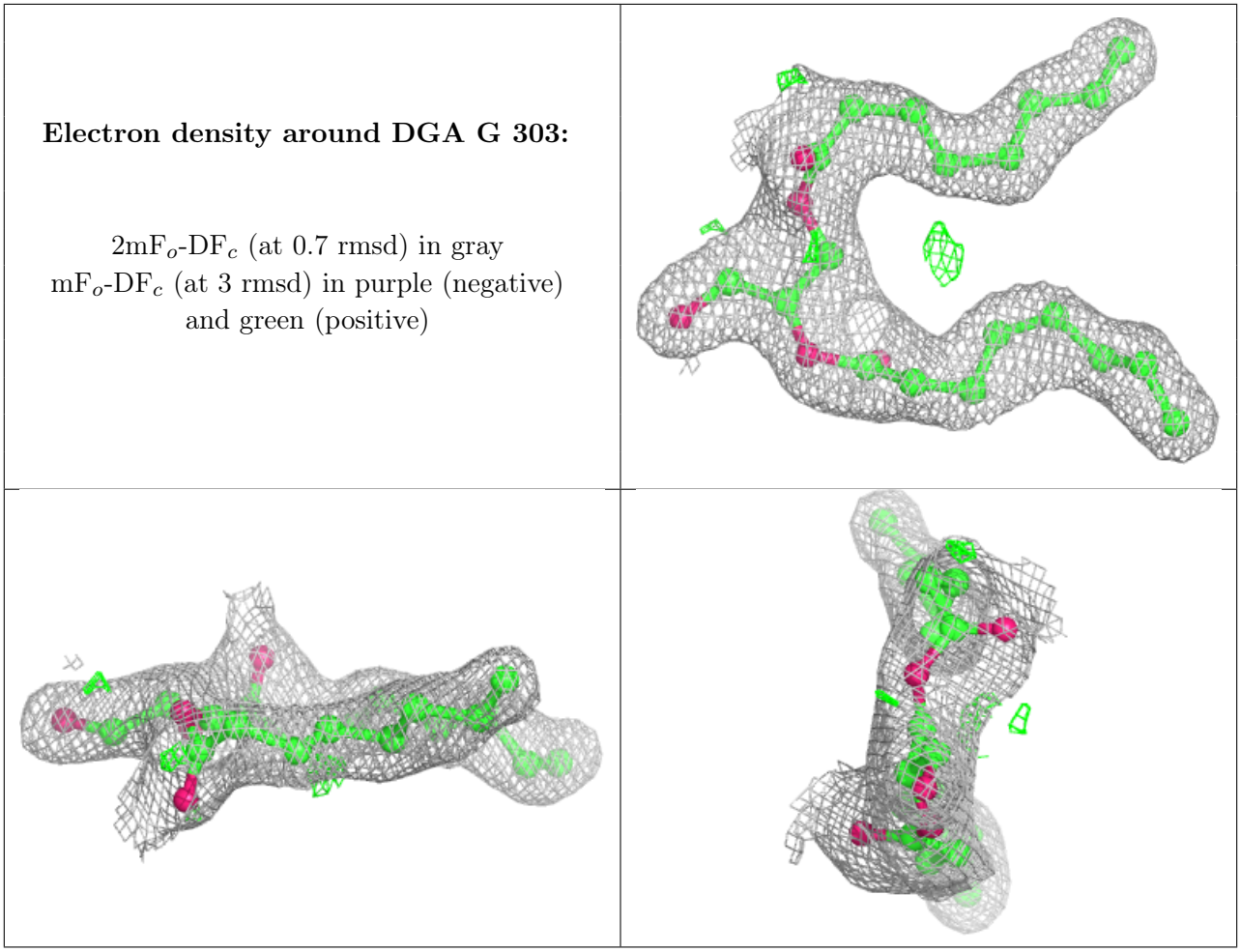
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





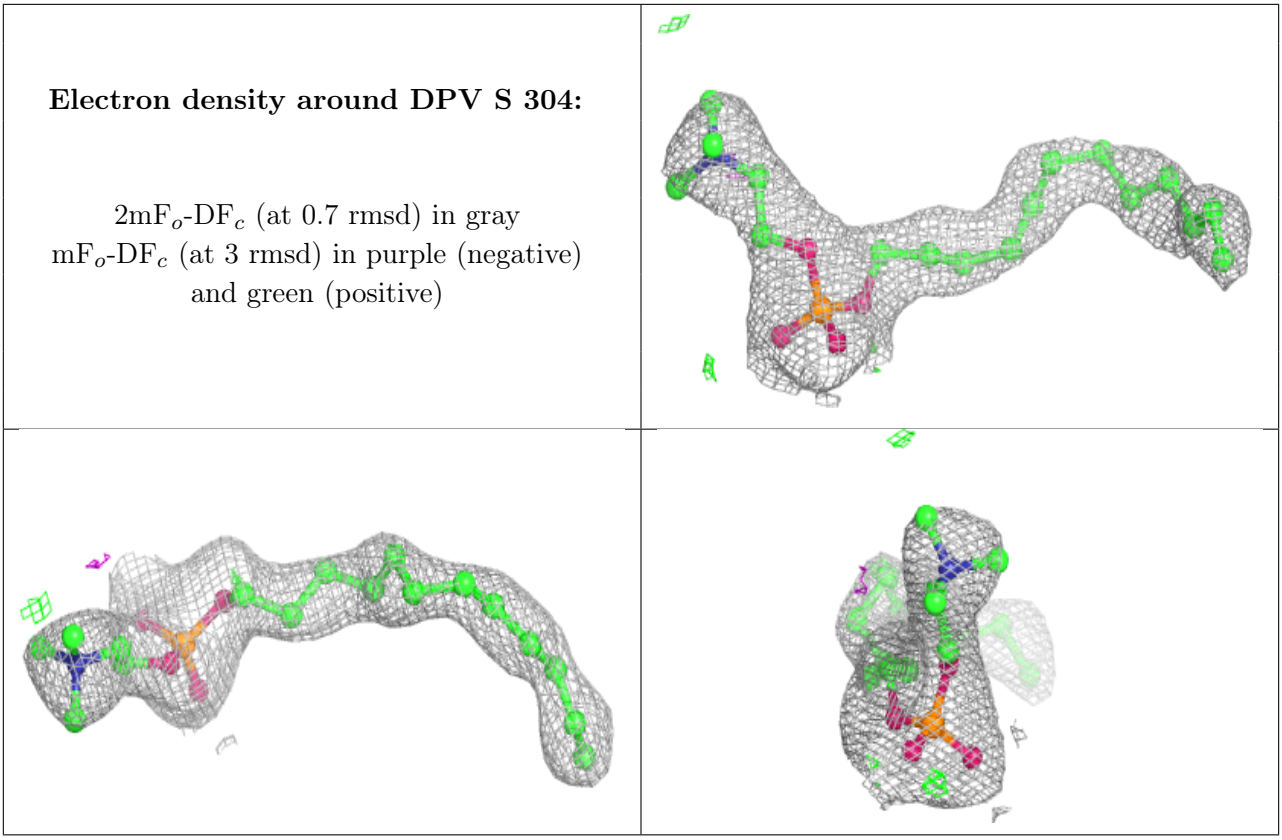
Electron density around DGA G 303:

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



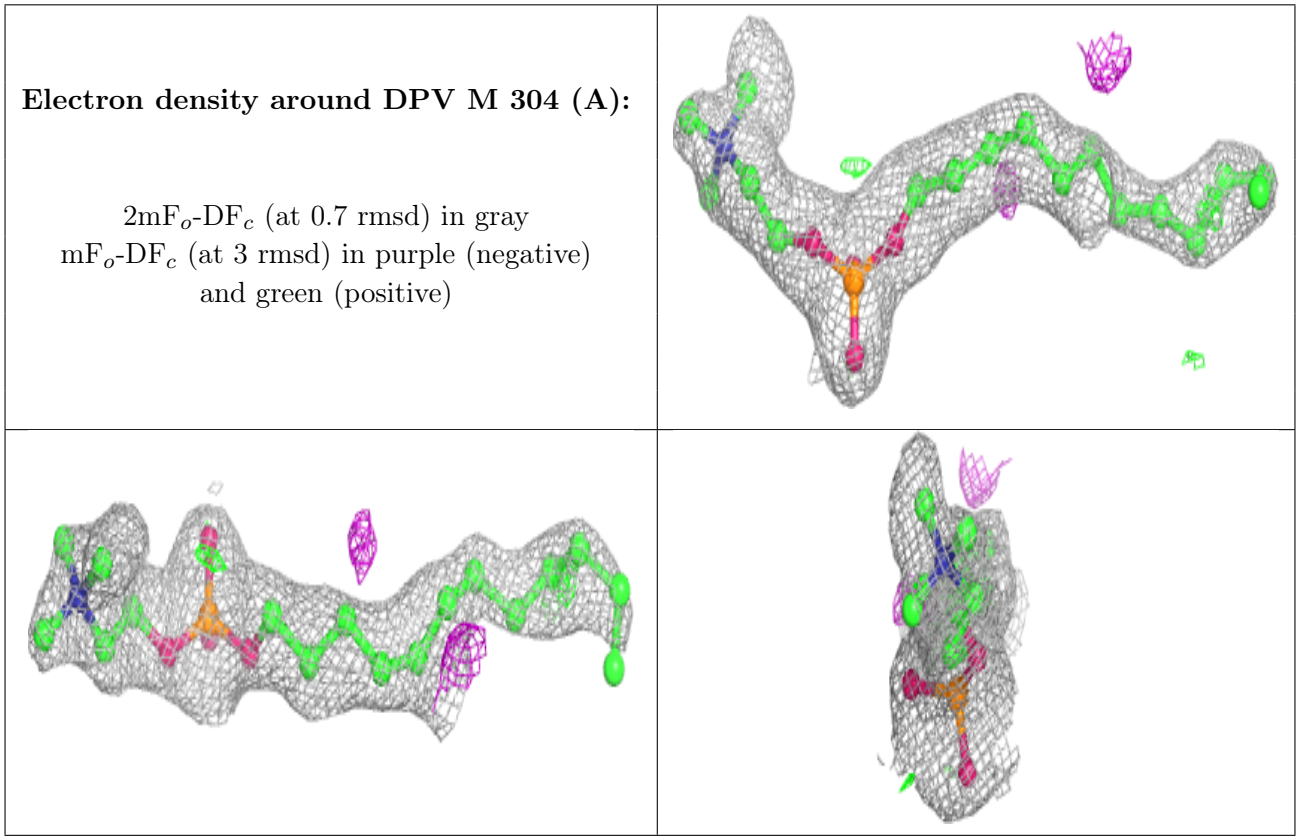
Electron density around DPV S 304:

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



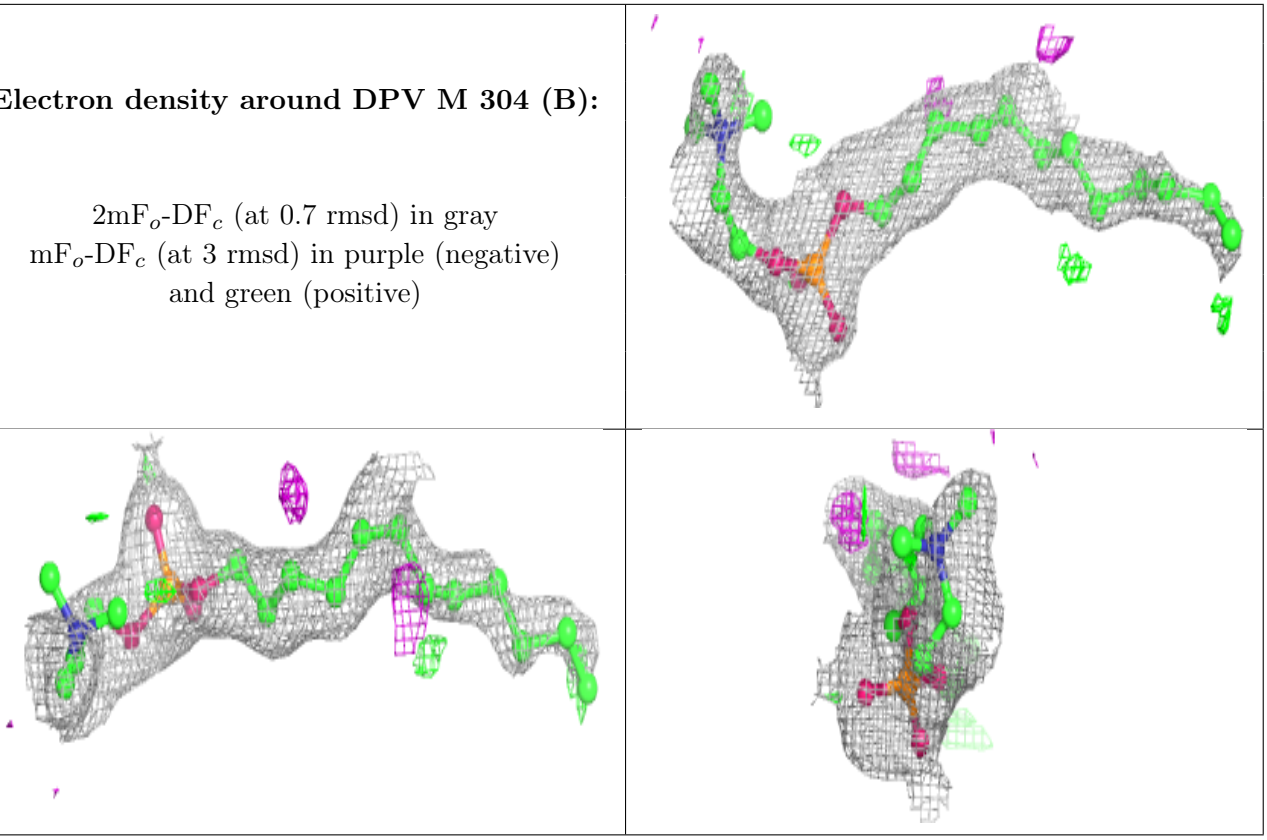
Electron density around DPV M 304 (A):

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



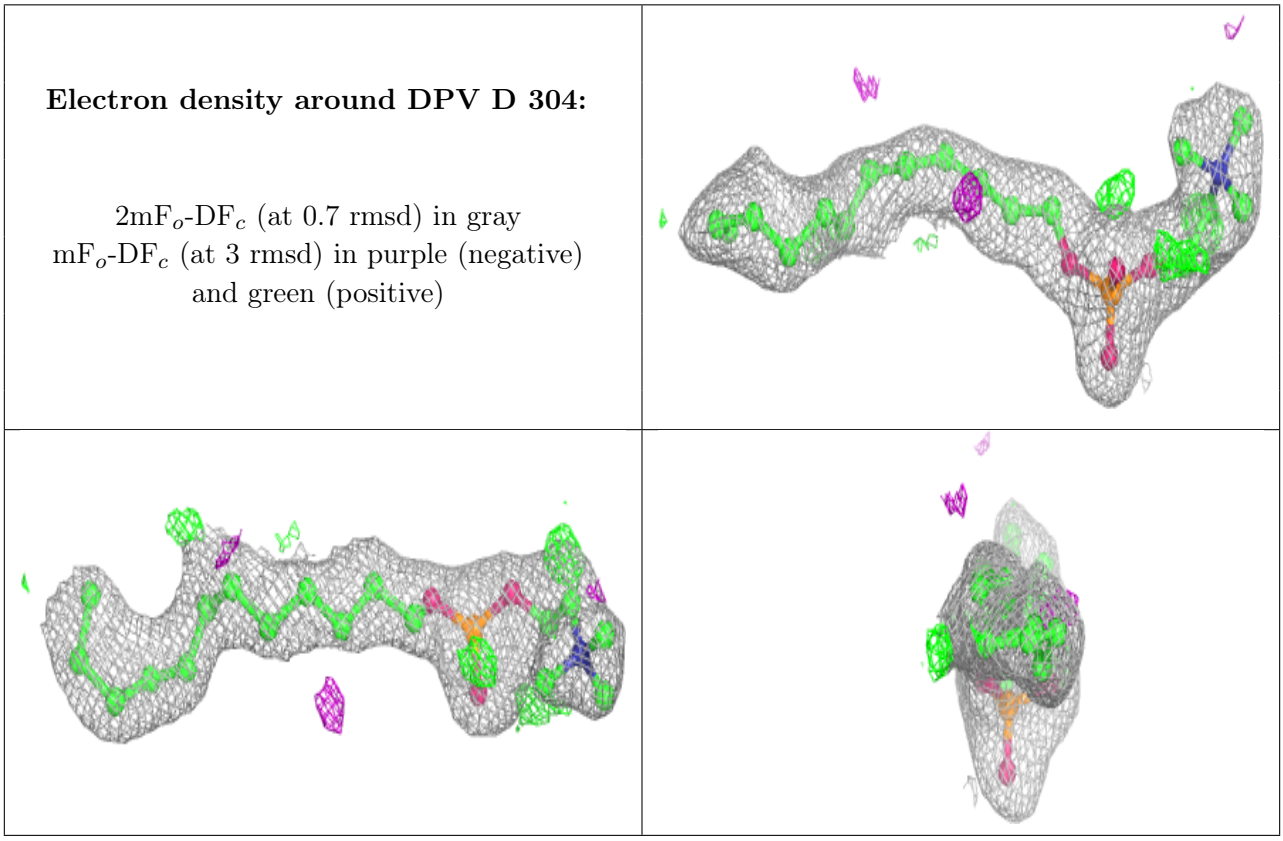
Electron density around DPV M 304 (B):

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



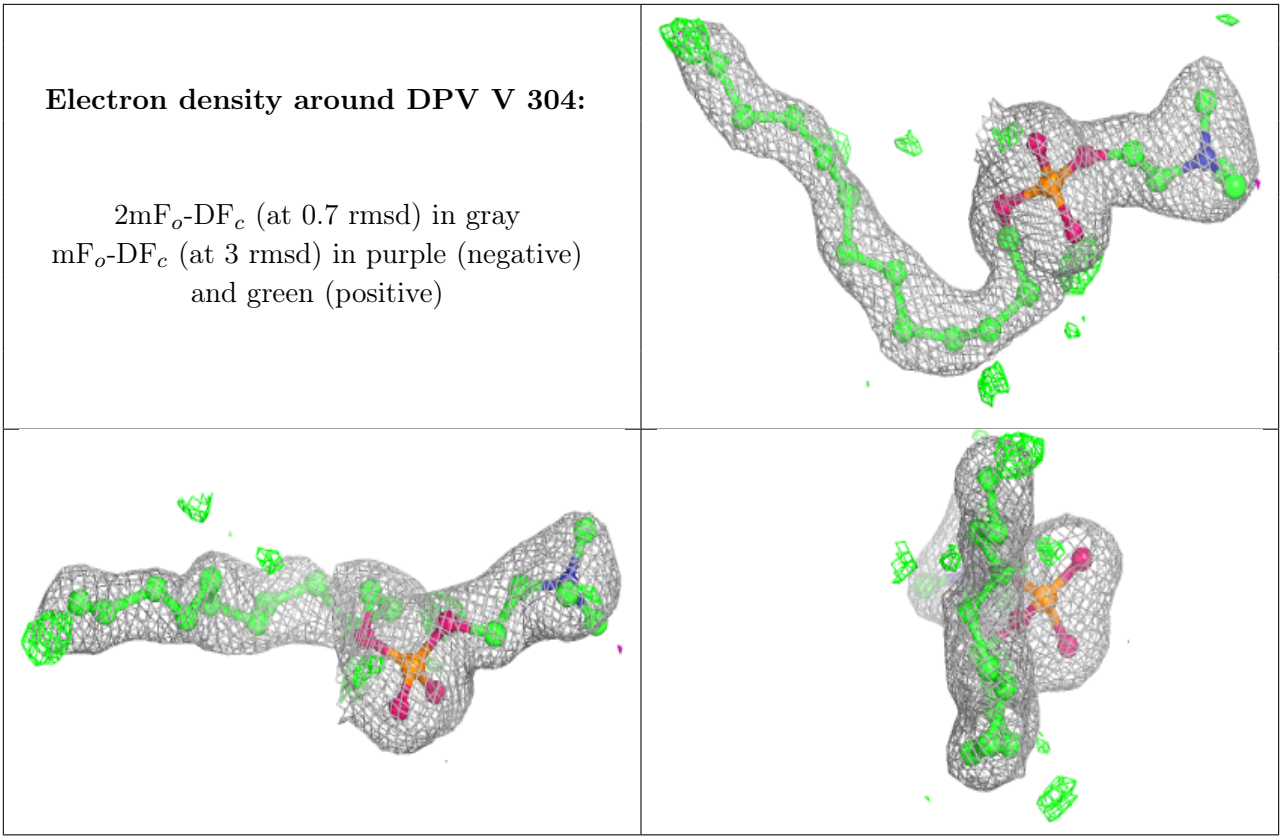
Electron density around DPV D 304:

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



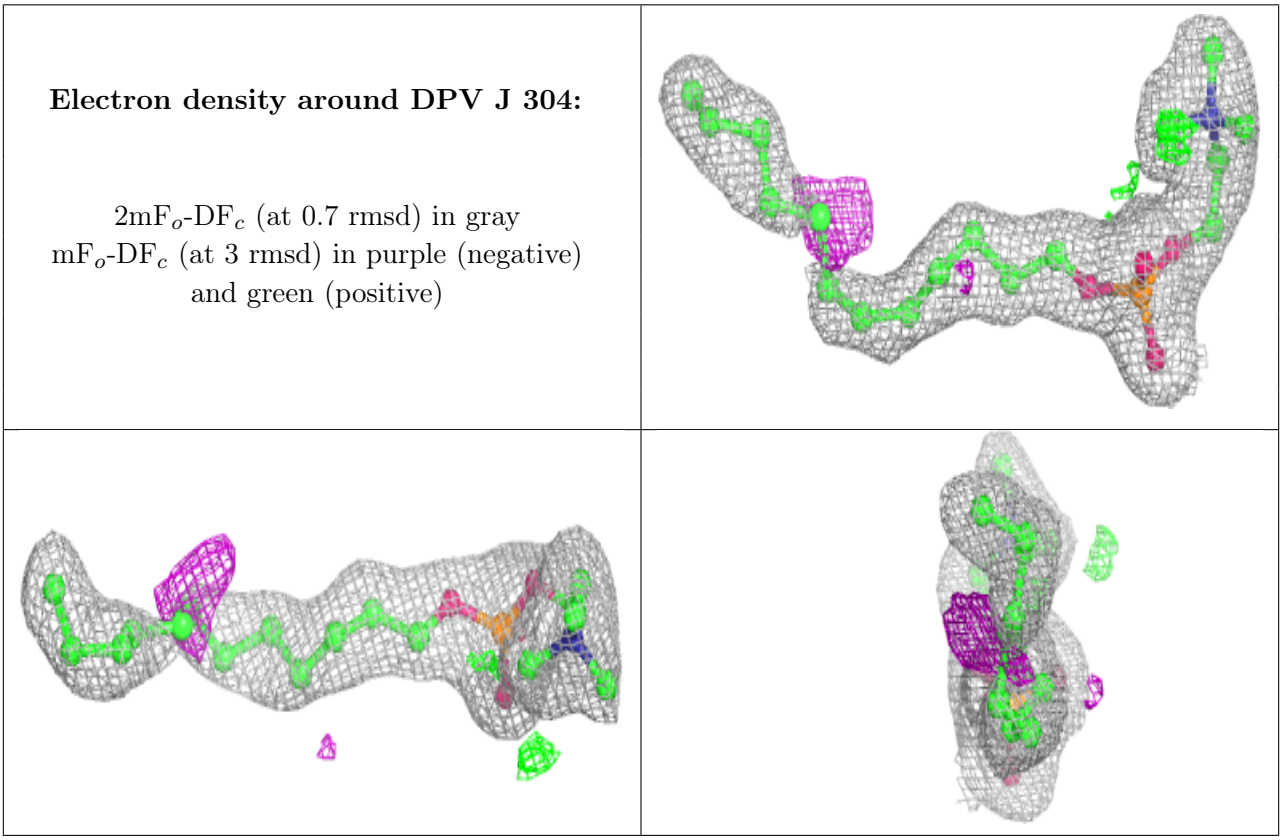
Electron density around DPV V 304:

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



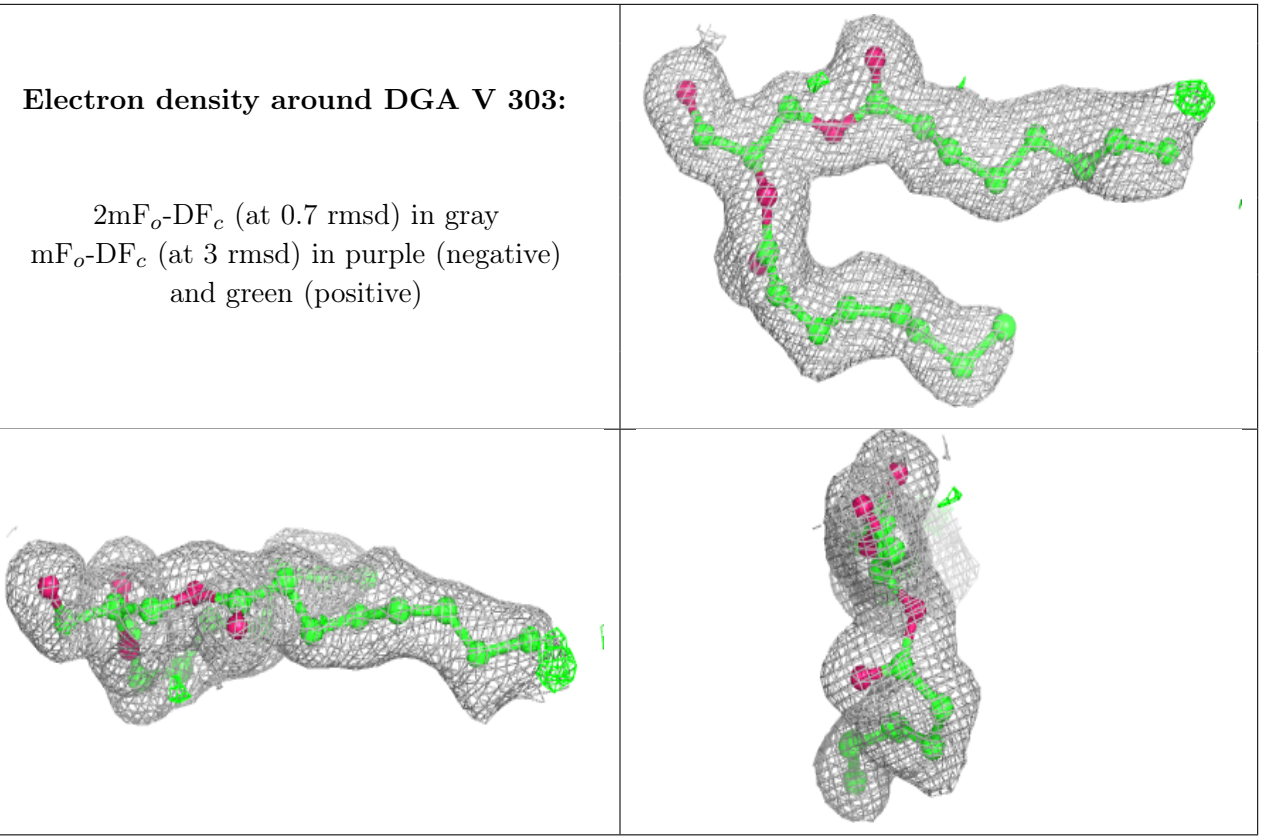
Electron density around DPV J 304:

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



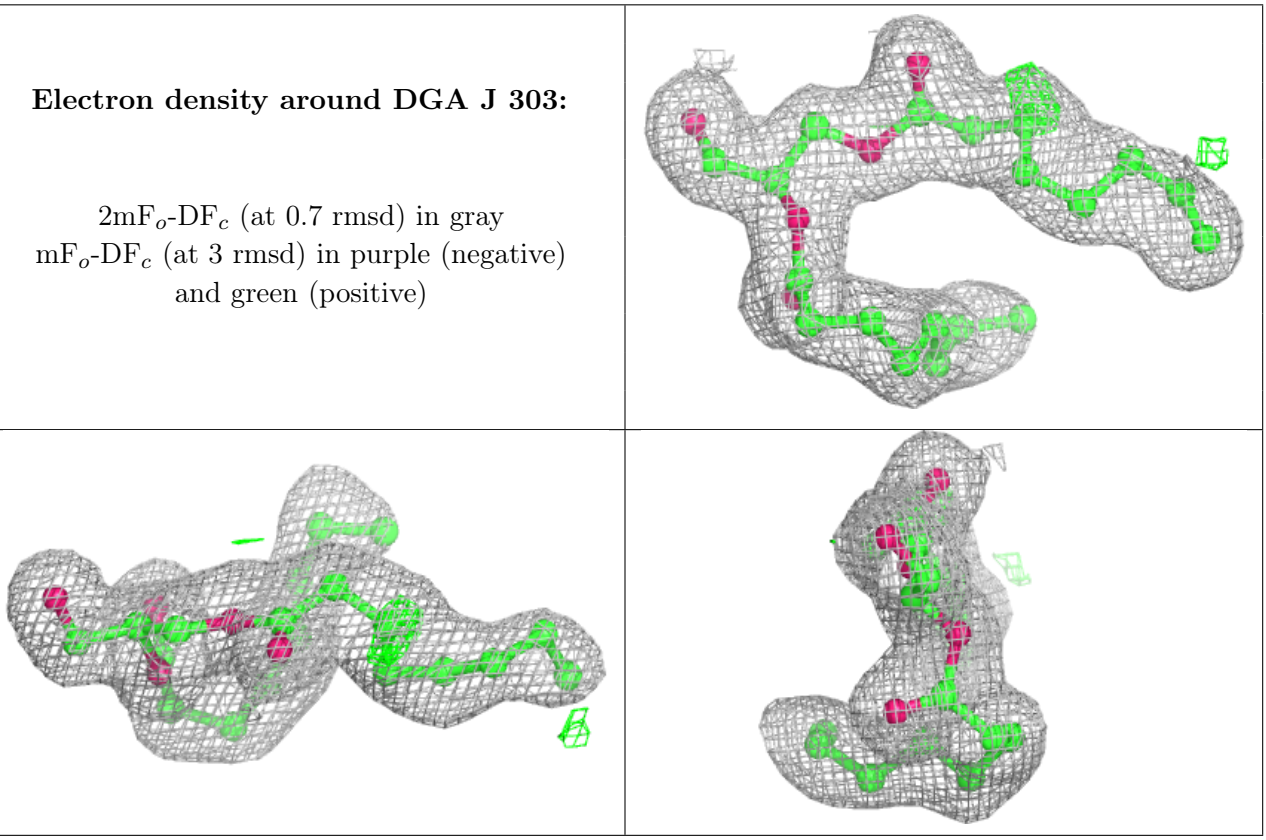
Electron density around DGA V 303:

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



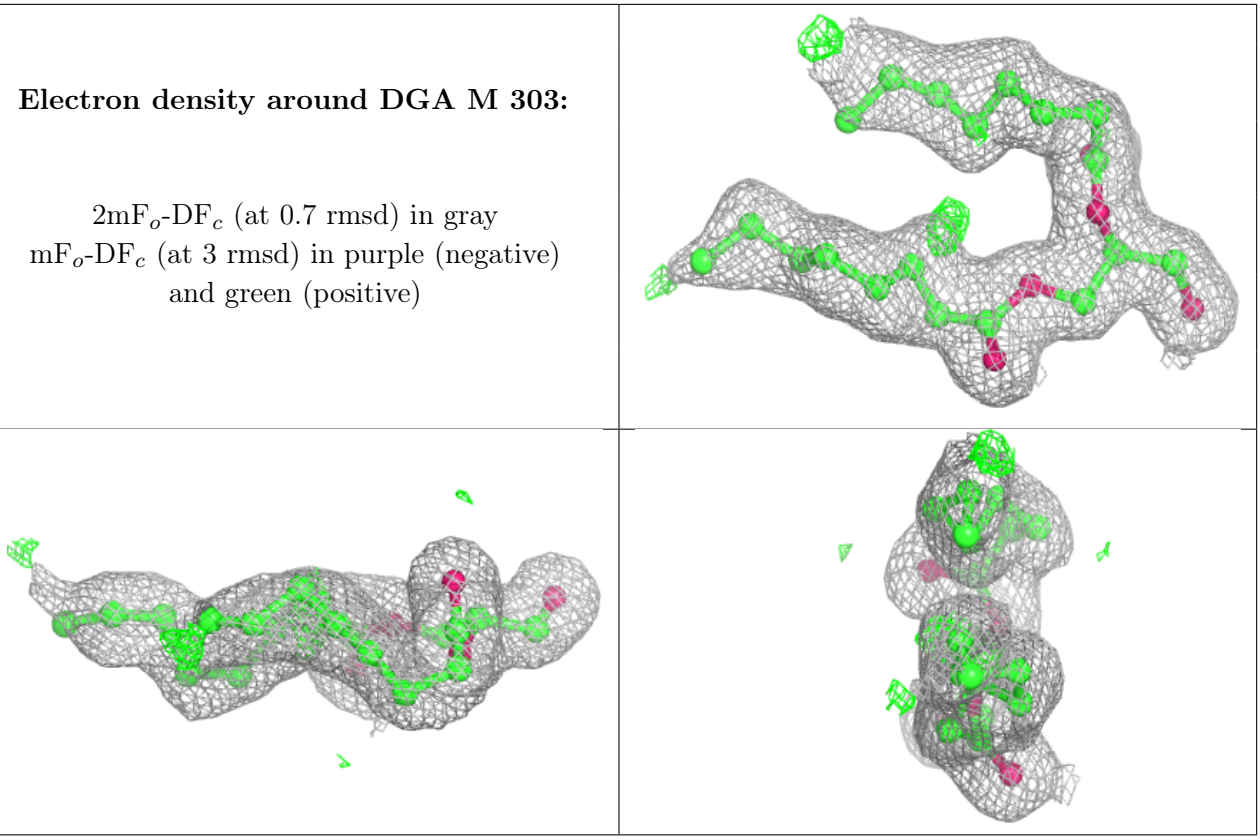
Electron density around DGA J 303:

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



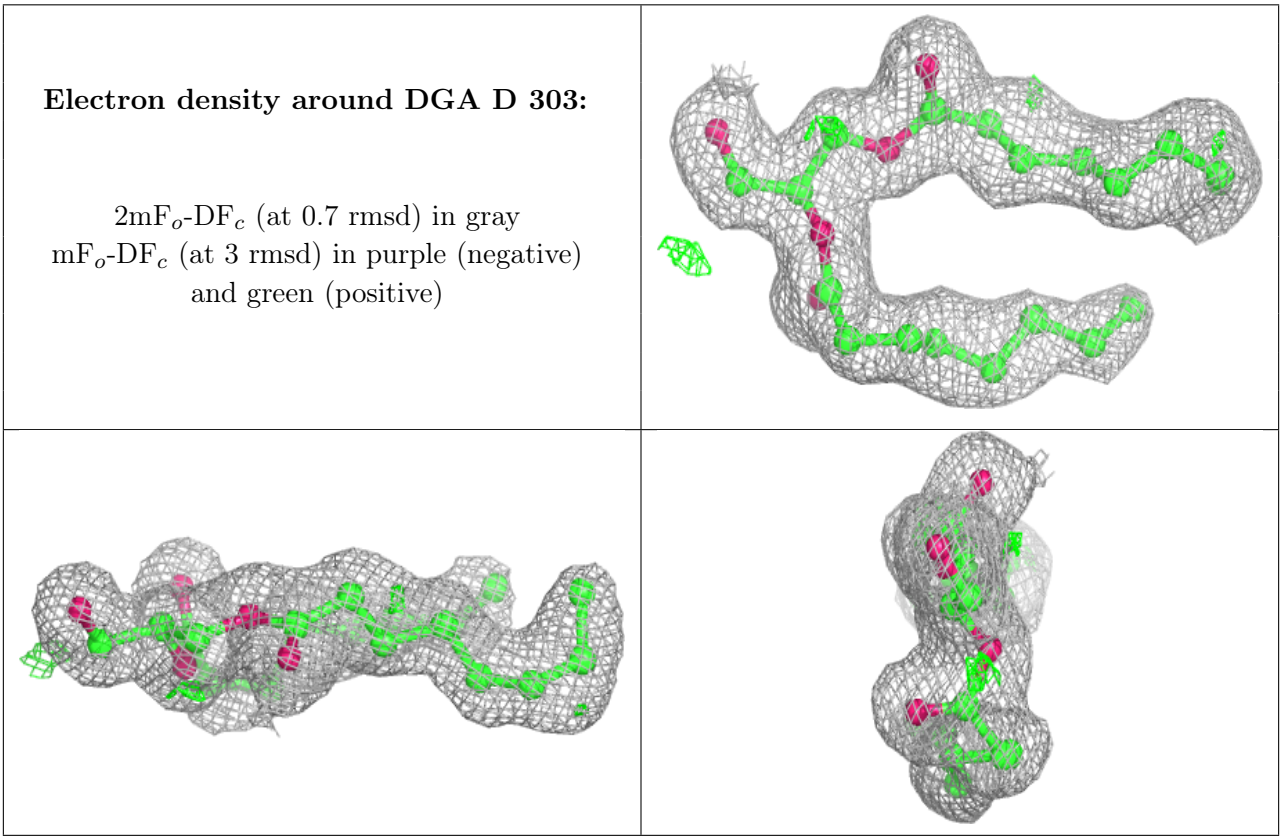
Electron density around DGA M 303:

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



Electron density around DGA D 303:

$2mF_o$-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.