



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:59 AM BST

PDB ID : 3VJC
Title : Crystal structure of the human squalene synthase in complex with zaragozic acid A
Authors : Liu, C.I.; Jeng, W.Y.; Chang, W.J.; Ko, T.P.; Wang, A.H.J.
Deposited on : 2011-10-14
Resolution : 1.89 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 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 : 2.13.1
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) : 2.13.1

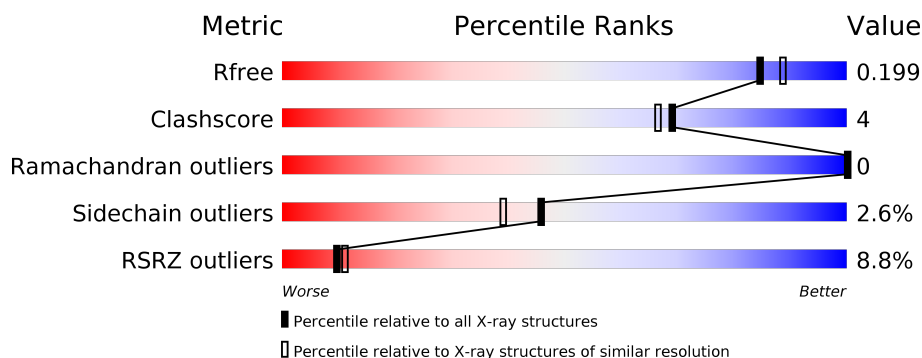
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	343	<div> <div>4%</div> <div>89%</div> <div>6%</div> <div>• •</div> </div>
1	B	343	<div> <div>3%</div> <div>90%</div> <div>6%</div> <div>• •</div> </div>
1	C	343	<div> <div>3%</div> <div>91%</div> <div>5%</div> <div>• •</div> </div>
1	D	343	<div> <div>9%</div> <div>88%</div> <div>8%</div> <div>• •</div> </div>
1	E	343	<div> <div>11%</div> <div>91%</div> <div>6%</div> <div>• •</div> </div>
1	F	343	<div> <div>20%</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 17855 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 Squalene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2699	1717	460	504	18			
1	B	333	Total	C	N	O	S	0	0	0
			2691	1711	459	503	18			
1	C	332	Total	C	N	O	S	0	0	0
			2682	1706	457	501	18			
1	D	333	Total	C	N	O	S	0	0	0
			2691	1711	459	503	18			
1	E	333	Total	C	N	O	S	0	0	0
			2691	1711	459	503	18			
1	F	332	Total	C	N	O	S	0	0	0
			2685	1708	458	501	18			

There are 18 discrepancies between the modelled and reference sequences:

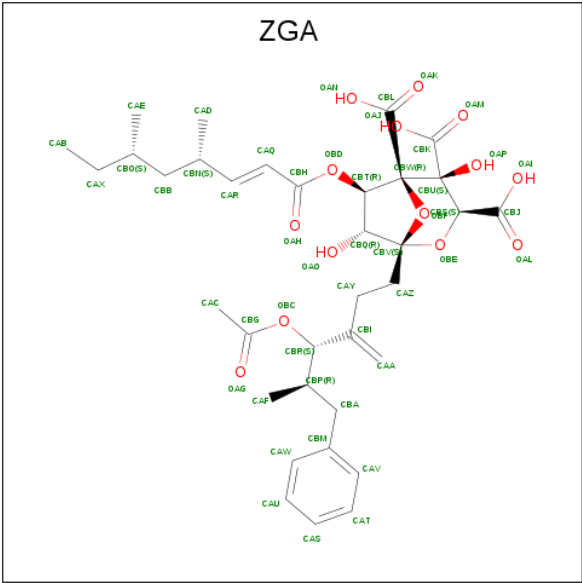
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLY	-	EXPRESSION TAG	UNP P37268
A	29	SER	-	EXPRESSION TAG	UNP P37268
A	30	HIS	-	EXPRESSION TAG	UNP P37268
B	28	GLY	-	EXPRESSION TAG	UNP P37268
B	29	SER	-	EXPRESSION TAG	UNP P37268
B	30	HIS	-	EXPRESSION TAG	UNP P37268
C	28	GLY	-	EXPRESSION TAG	UNP P37268
C	29	SER	-	EXPRESSION TAG	UNP P37268
C	30	HIS	-	EXPRESSION TAG	UNP P37268
D	28	GLY	-	EXPRESSION TAG	UNP P37268
D	29	SER	-	EXPRESSION TAG	UNP P37268
D	30	HIS	-	EXPRESSION TAG	UNP P37268
E	28	GLY	-	EXPRESSION TAG	UNP P37268
E	29	SER	-	EXPRESSION TAG	UNP P37268
E	30	HIS	-	EXPRESSION TAG	UNP P37268
F	28	GLY	-	EXPRESSION TAG	UNP P37268
F	29	SER	-	EXPRESSION TAG	UNP P37268

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Chain	Residue	Modelled	Actual	Comment	Reference
F	30	HIS	-	EXPRESSION TAG	UNP P37268

- Molecule 2 is Zaragozic acid A (three-letter code: ZGA) (formula: C₃₅H₄₆O₁₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 49 35 14	0	0
2	B	1	Total C O 49 35 14	0	0
2	C	1	Total C O 49 35 14	0	0
2	D	1	Total C O 49 35 14	0	0
2	E	1	Total C O 49 35 14	0	0
2	F	1	Total C O 49 35 14	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	354	Total	O	0	0
			354	354		

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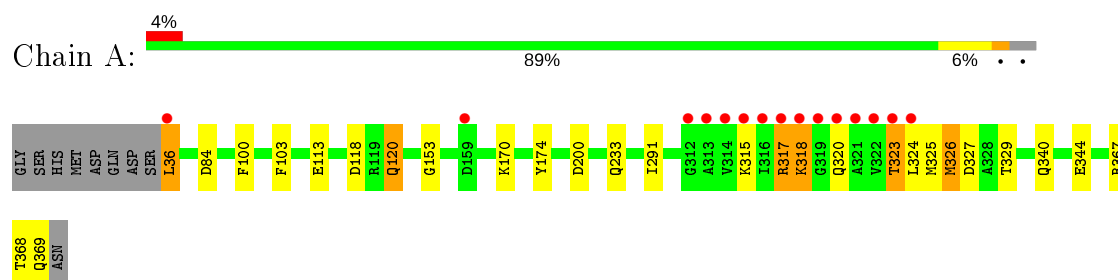
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	318	Total 318	O 318	0	0
5	C	330	Total 330	O 330	0	0
5	D	138	Total 138	O 138	0	0
5	E	180	Total 180	O 180	0	0
5	F	70	Total 70	O 70	0	0

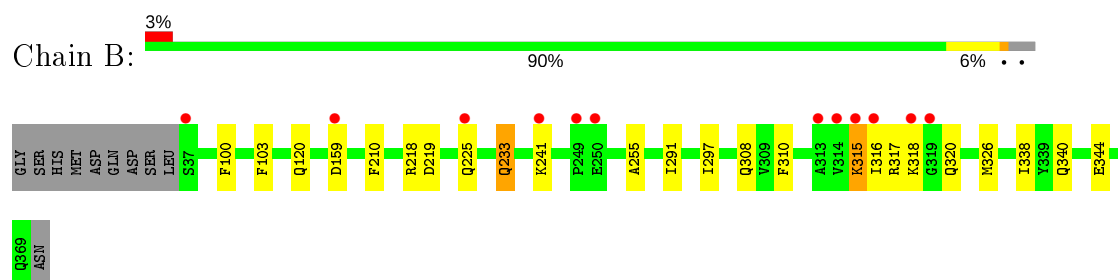
3 Residue-property plots

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.

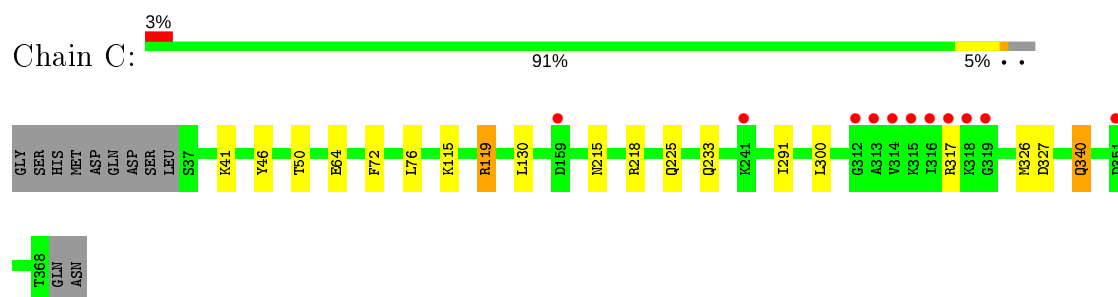
• Molecule 1: Squalene synthase



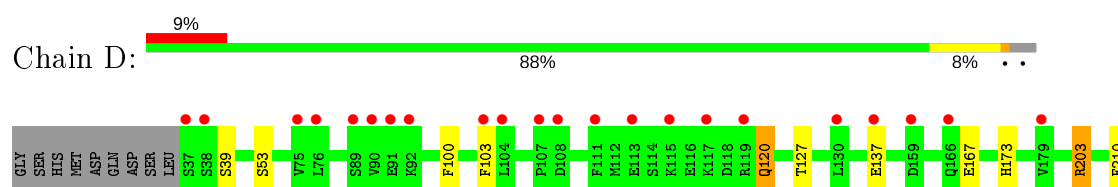
• Molecule 1: Squalene synthase

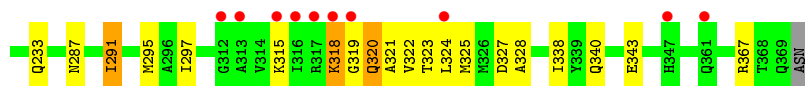


• Molecule 1: Squalene synthase

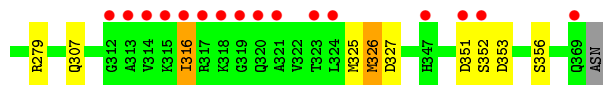
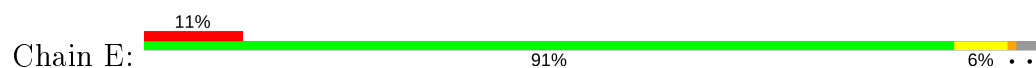


• Molecule 1: Squalene synthase

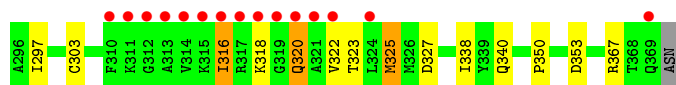
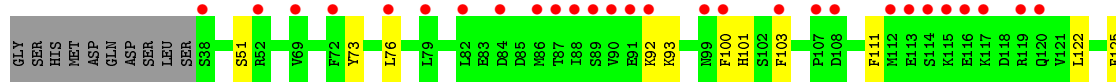
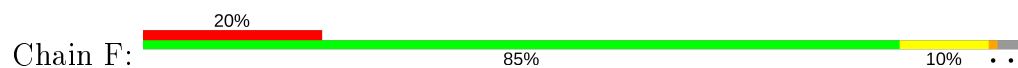




• Molecule 1: Squalene synthase



• Molecule 1: Squalene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.87Å 153.15Å 91.86Å 90.00° 91.72° 90.00°	Depositor
Resolution (Å)	27.70 – 1.89 27.65 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.4 (27.70-1.89) 99.3 (27.65-1.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.148 , 0.197 0.148 , 0.199	Depositor DCC
R_{free} test set	9433 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17855	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZGA, PO4, MG

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	0.43	0/2754	0.69	1/3724 (0.0%)
1	B	0.38	0/2746	0.65	0/3713
1	C	0.40	0/2737	0.70	2/3701 (0.1%)
1	D	0.30	0/2746	0.61	0/3713
1	E	0.34	0/2746	0.61	0/3713
1	F	0.27	0/2740	0.55	0/3705
All	All	0.36	0/16469	0.64	3/22269 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	C	64	GLU	CB-CA-C	-5.90	98.60	110.40
1	C	300	LEU	CA-CB-CG	5.29	127.47	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2699	0	2680	29	0
1	B	2691	0	2669	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2682	0	2661	14	0
1	D	2691	0	2669	32	0
1	E	2691	0	2669	14	0
1	F	2685	0	2664	25	0
2	A	49	0	43	0	0
2	B	49	0	43	0	0
2	C	49	0	43	1	0
2	D	49	0	43	4	0
2	E	49	0	43	1	0
2	F	49	0	43	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	354	0	0	9	0
5	B	318	0	0	1	0
5	C	330	0	0	2	0
5	D	138	0	0	3	0
5	E	180	0	0	1	0
5	F	70	0	0	0	0
All	All	17855	0	16270	120	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 4.

All (120) 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:315:LYS:HD3	1:B:315:LYS:H	1.25	1.01
1:D:320:GLN:HE21	1:D:340:GLN:HE22	1.07	0.96
2:C:400:ZGA:HABB	2:C:400:ZGA:HBN	1.56	0.86
1:A:200:ASP:HB3	5:A:1198:HOH:O	1.79	0.82
1:A:317:ARG:HH21	1:A:317:ARG:HG3	1.46	0.80
1:D:320:GLN:NE2	1:D:340:GLN:HE22	1.80	0.79
1:A:340:GLN:HG2	5:A:1639:HOH:O	1.86	0.74
1:D:320:GLN:HE21	1:D:340:GLN:NE2	1.83	0.74
1:A:326:MET:HE3	1:C:291:ILE:HD11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLN:HG3	5:A:1699:HOH:O	1.90	0.72
1:A:120:GLN:CG	5:A:1699:HOH:O	2.39	0.70
1:B:297:ILE:HD13	1:B:338:ILE:HG12	1.74	0.68
1:A:344:GLU:HG3	5:A:1265:HOH:O	1.95	0.67
1:A:120:GLN:H	1:A:120:GLN:CD	1.99	0.66
1:D:167:GLU:HG2	5:D:1552:HOH:O	1.94	0.66
1:A:323:THR:HG22	1:A:324:LEU:HG	1.78	0.66
1:D:203:ARG:NH2	5:D:886:HOH:O	2.19	0.65
1:A:317:ARG:NH2	1:A:317:ARG:HG3	2.11	0.64
1:D:297:ILE:HD13	1:D:338:ILE:HG12	1.80	0.64
1:D:53:SER:CB	2:D:400:ZGA:HAQ	2.29	0.62
1:A:323:THR:HA	1:A:340:GLN:OE1	1.99	0.62
1:D:320:GLN:HE22	1:D:322:VAL:HB	1.65	0.61
1:D:323:THR:HG23	1:D:340:GLN:CD	2.21	0.61
1:F:323:THR:HG21	1:F:340:GLN:HG3	1.83	0.60
1:D:100:PHE:HA	1:D:103:PHE:CD2	2.37	0.60
1:E:233:GLN:HA	1:E:236:TRP:NE1	2.16	0.60
1:D:295:MET:HB2	2:D:400:ZGA:HAEA	1.85	0.58
1:D:320:GLN:HB3	1:D:340:GLN:OE1	2.03	0.58
1:A:170:LYS:HE2	1:A:174:TYR:OH	2.03	0.58
1:D:318:LYS:HD2	1:D:319:GLY:N	2.19	0.57
1:A:326:MET:HE3	1:C:291:ILE:CD1	2.33	0.57
1:A:368:THR:HG21	1:C:41:LYS:HA	1.87	0.56
1:F:323:THR:CG2	1:F:340:GLN:HG3	2.34	0.56
1:A:369:GLN:HA	1:A:369:GLN:OE1	2.06	0.56
1:A:323:THR:CA	1:A:340:GLN:OE1	2.53	0.56
1:F:125:PHE:N	1:F:126:PRO:HD2	2.21	0.55
1:A:36:LEU:N	5:A:1418:HOH:O	2.40	0.55
1:F:150:MET:HG3	1:F:174:TYR:O	2.07	0.55
1:E:316:ILE:H	1:E:316:ILE:HD13	1.72	0.54
1:F:215:ASN:HD21	2:F:400:ZGA:HAX	1.73	0.54
1:D:343:GLU:OE1	1:D:367:ARG:NH2	2.41	0.54
1:D:320:GLN:NE2	1:D:322:VAL:HB	2.23	0.53
1:B:159:ASP:HB2	5:B:1348:HOH:O	2.08	0.53
1:D:39:SER:HB2	1:D:127:THR:HG23	1.91	0.53
1:A:318:LYS:HE3	1:A:318:LYS:N	2.24	0.53
1:B:210:PHE:HE2	1:B:297:ILE:HG13	1.73	0.53
1:B:315:LYS:N	1:B:315:LYS:HD3	2.10	0.52
1:D:327:ASP:HB2	1:E:325:MET:O	2.10	0.52
1:D:210:PHE:CE2	1:D:297:ILE:HG13	2.45	0.52
1:A:118:ASP:HA	1:A:120:GLN:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:PHE:CE2	1:B:297:ILE:HG13	2.45	0.51
1:F:320:GLN:HB3	1:F:340:GLN:OE1	2.10	0.51
1:E:66:ARG:NH1	1:F:367:ARG:O	2.40	0.51
1:C:327:ASP:OD2	5:C:1758:HOH:O	2.19	0.51
1:C:215:ASN:OD1	1:C:218:ARG:NH2	2.43	0.50
1:E:252:ILE:HD11	1:E:307:GLN:HB2	1.92	0.50
1:A:100:PHE:HA	1:A:103:PHE:CD2	2.47	0.50
1:A:318:LYS:HE3	1:A:318:LYS:H	1.77	0.50
1:F:150:MET:O	1:F:154:MET:HG3	2.12	0.50
1:F:101:HIS:CD2	1:F:148:ARG:HG3	2.48	0.49
1:F:320:GLN:HE22	1:F:322:VAL:HB	1.78	0.49
1:F:51:SER:HB2	1:F:73:TYR:CZ	2.47	0.49
1:B:100:PHE:HA	1:B:103:PHE:CD2	2.47	0.49
1:F:100:PHE:HA	1:F:103:PHE:CD2	2.47	0.49
1:D:321:ALA:HA	1:D:324:LEU:HD12	1.94	0.48
1:F:316:ILE:H	1:F:316:ILE:HD13	1.78	0.48
1:B:297:ILE:CD1	1:B:338:ILE:HG12	2.43	0.48
1:E:233:GLN:HA	1:E:236:TRP:CD1	2.49	0.48
1:F:350:PRO:HG2	1:F:353:ASP:HB2	1.96	0.48
1:D:120:GLN:HG3	1:D:120:GLN:H	1.40	0.48
1:F:76:LEU:HD12	2:F:400:ZGA:HAV	1.96	0.48
1:A:326:MET:CE	1:C:291:ILE:CD1	2.92	0.47
1:D:325:MET:O	1:F:327:ASP:HB2	2.13	0.47
1:C:130:LEU:HD12	5:C:950:HOH:O	2.14	0.47
1:B:308:GLN:HG3	1:B:315:LYS:HE3	1.96	0.47
1:D:53:SER:HB2	2:D:400:ZGA:HAQ	1.95	0.47
1:D:137:GLU:HA	5:D:1732:HOH:O	2.15	0.47
1:A:325:MET:O	1:C:327:ASP:HB2	2.16	0.46
1:F:93:LYS:HE3	1:F:158:LEU:HD11	1.98	0.46
1:D:287:ASN:HB3	1:E:326:MET:HE1	1.95	0.46
1:A:153:GLY:HA3	1:A:174:TYR:CG	2.51	0.46
1:A:291:ILE:HD11	1:B:326:MET:CG	2.45	0.46
1:E:66:ARG:NH2	5:E:1441:HOH:O	2.48	0.46
1:B:291:ILE:CD1	1:C:326:MET:HE3	2.46	0.46
1:E:211:LEU:HD22	2:E:400:ZGA:HAEB	1.98	0.45
1:A:329:THR:HG21	5:A:1260:HOH:O	2.17	0.44
1:B:255:ALA:HB1	1:B:310:PHE:CZ	2.52	0.44
1:F:291:ILE:O	1:F:295:MET:HG3	2.18	0.44
1:B:233:GLN:HE21	1:B:233:GLN:HB3	1.61	0.43
1:D:210:PHE:HE2	1:D:297:ILE:HG13	1.83	0.43
1:E:353:ASP:O	1:E:356:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:ARG:HD3	1:D:203:ARG:N	2.33	0.43
1:D:291:ILE:HD12	1:D:328:ALA:HB3	2.01	0.43
1:C:340:GLN:HB3	1:C:340:GLN:HE21	1.60	0.43
1:C:72:PHE:CZ	1:C:76:LEU:HD11	2.54	0.43
1:E:100:PHE:HD2	1:E:147:CYS:SG	2.43	0.42
1:F:111:PHE:HB3	1:F:122:LEU:HB3	2.01	0.42
1:B:316:ILE:HD12	1:B:316:ILE:N	2.33	0.42
1:A:120:GLN:CD	5:A:1699:HOH:O	2.57	0.42
1:B:218:ARG:HD2	1:B:219:ASP:OD1	2.19	0.42
1:D:321:ALA:O	1:D:324:LEU:HB2	2.19	0.42
1:A:327:ASP:OD2	5:A:1260:HOH:O	2.22	0.42
1:F:297:ILE:HD13	1:F:338:ILE:HG12	2.02	0.42
1:E:327:ASP:HB2	1:F:325:MET:O	2.19	0.42
1:B:315:LYS:H	1:B:315:LYS:CD	2.05	0.41
1:F:297:ILE:CD1	1:F:338:ILE:HG12	2.51	0.41
1:D:173:HIS:NE2	3:D:401:PO4:O3	2.53	0.41
1:F:125:PHE:N	1:F:126:PRO:CD	2.83	0.41
1:F:259:LEU:HD21	1:F:303:CYS:O	2.21	0.41
1:C:46:TYR:O	1:C:50:THR:HG23	2.20	0.41
1:E:196:LEU:HD21	1:E:279:ARG:CZ	2.50	0.41
1:A:368:THR:HG21	1:C:41:LYS:HG2	2.02	0.41
2:D:400:ZGA:HBB	2:D:400:ZGA:HABB	1.73	0.41
1:D:315:LYS:HA	1:D:315:LYS:HD2	1.78	0.41
1:F:101:HIS:CG	1:F:148:ARG:HG3	2.55	0.41
1:B:340:GLN:O	1:B:344:GLU:HG2	2.20	0.40
1:C:115:LYS:NZ	1:C:119:ARG:HH22	2.19	0.40
1:D:323:THR:HG23	1:D:340:GLN:OE1	2.21	0.40
1:E:163:THR:HG22	1:E:233:GLN:HE21	1.86	0.40
1:D:323:THR:CG2	1:D:340:GLN:CD	2.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/343 (97%)	327 (98%)	5 (2%)	0	100	100
1	B	331/343 (96%)	327 (99%)	4 (1%)	0	100	100
1	C	330/343 (96%)	325 (98%)	5 (2%)	0	100	100
1	D	331/343 (96%)	323 (98%)	8 (2%)	0	100	100
1	E	331/343 (96%)	327 (99%)	4 (1%)	0	100	100
1	F	330/343 (96%)	322 (98%)	8 (2%)	0	100	100
All	All	1985/2058 (96%)	1951 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/305 (97%)	286 (96%)	11 (4%)	34	25
1	B	296/305 (97%)	288 (97%)	8 (3%)	44	38
1	C	295/305 (97%)	290 (98%)	5 (2%)	60	57
1	D	296/305 (97%)	290 (98%)	6 (2%)	55	51
1	E	296/305 (97%)	290 (98%)	6 (2%)	55	51
1	F	295/305 (97%)	284 (96%)	11 (4%)	34	25
All	All	1775/1830 (97%)	1728 (97%)	47 (3%)	46	39

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	84	ASP
1	A	113	GLU
1	A	120	GLN
1	A	233	GLN
1	A	315	LYS
1	A	317	ARG

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Mol	Chain	Res	Type
1	A	318	LYS
1	A	320	GLN
1	A	323	THR
1	A	326	MET
1	B	120	GLN
1	B	225	GLN
1	B	233	GLN
1	B	241	LYS
1	B	315	LYS
1	B	317	ARG
1	B	318	LYS
1	B	320	GLN
1	C	119	ARG
1	C	225	GLN
1	C	233	GLN
1	C	317	ARG
1	C	340	GLN
1	D	120	GLN
1	D	203	ARG
1	D	233	GLN
1	D	291	ILE
1	D	318	LYS
1	D	320	GLN
1	E	83	GLU
1	E	225	GLN
1	E	316	ILE
1	E	326	MET
1	E	351	ASP
1	E	352	SER
1	F	92	LYS
1	F	158	LEU
1	F	159	ASP
1	F	162	VAL
1	F	166	GLN
1	F	218	ARG
1	F	233	GLN
1	F	316	ILE
1	F	318	LYS
1	F	320	GLN
1	F	325	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	A	233	GLN
1	A	257	GLN
1	A	283	GLN
1	A	308	GLN
1	B	120	GLN
1	B	225	GLN
1	B	233	GLN
1	B	257	GLN
1	B	340	GLN
1	B	347	HIS
1	B	369	GLN
1	C	233	GLN
1	C	340	GLN
1	D	101	HIS
1	D	140	GLN
1	D	166	GLN
1	D	225	GLN
1	D	233	GLN
1	D	257	GLN
1	D	320	GLN
1	E	49	GLN
1	E	120	GLN
1	E	233	GLN
1	F	215	ASN
1	F	225	GLN
1	F	257	GLN
1	F	283	GLN
1	F	320	GLN
1	F	340	GLN
1	F	369	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	PO4	C	401	-	4,4,4	1.02	0	6,6,6	0.91	0
3	PO4	B	401	-	4,4,4	0.88	0	6,6,6	0.74	0
3	PO4	E	401	-	4,4,4	0.97	0	6,6,6	1.09	0
2	ZGA	E	400	-	38,51,51	1.26	2 (5%)	36,76,76	1.50	4 (11%)
3	PO4	F	401	-	4,4,4	0.90	0	6,6,6	0.31	0
2	ZGA	D	400	-	38,51,51	1.25	2 (5%)	36,76,76	1.16	5 (13%)
2	ZGA	A	400	-	38,51,51	1.26	2 (5%)	36,76,76	1.52	4 (11%)
2	ZGA	F	400	-	38,51,51	1.29	2 (5%)	36,76,76	1.42	6 (16%)
2	ZGA	C	400	-	38,51,51	1.27	2 (5%)	36,76,76	1.42	6 (16%)
3	PO4	D	401	-	4,4,4	1.01	0	6,6,6	0.55	0
3	PO4	A	401	-	4,4,4	0.88	0	6,6,6	0.72	0
2	ZGA	B	400	-	38,51,51	1.29	2 (5%)	36,76,76	1.46	4 (11%)

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
2	ZGA	E	400	-	-	0/37/95/95	0/4/3/3
2	ZGA	D	400	-	-	5/37/95/95	0/4/3/3
2	ZGA	A	400	-	-	0/37/95/95	0/4/3/3
2	ZGA	F	400	-	-	4/37/95/95	0/4/3/3
2	ZGA	C	400	-	-	4/37/95/95	0/4/3/3
2	ZGA	B	400	-	-	1/37/95/95	0/4/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	400	ZGA	OBD-CBH	5.66	1.46	1.34
2	C	400	ZGA	OBD-CBH	5.60	1.46	1.34
2	B	400	ZGA	OBD-CBH	5.51	1.45	1.34
2	E	400	ZGA	OBD-CBH	5.41	1.45	1.34
2	D	400	ZGA	OBD-CBH	5.20	1.45	1.34
2	A	400	ZGA	OBD-CBH	5.11	1.45	1.34
2	D	400	ZGA	OBC-CBG	4.69	1.45	1.35
2	F	400	ZGA	OBC-CBG	4.68	1.45	1.35
2	E	400	ZGA	OBC-CBG	4.62	1.45	1.35
2	A	400	ZGA	OBC-CBG	4.59	1.45	1.35
2	B	400	ZGA	OBC-CBG	4.58	1.45	1.35
2	C	400	ZGA	OBC-CBG	4.24	1.44	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	ZGA	OBF-CBV-CBQ	-6.31	96.51	103.98
2	E	400	ZGA	OBC-CBG-CAC	5.17	120.61	111.09
2	A	400	ZGA	OBC-CBG-CAC	4.99	120.27	111.09
2	A	400	ZGA	OBF-CBV-CBQ	-4.11	99.11	103.98
2	C	400	ZGA	OBF-CBV-CBQ	-4.01	99.24	103.98
2	F	400	ZGA	OBC-CBG-CAC	3.88	118.24	111.09
2	A	400	ZGA	OBC-CBG-OAG	-3.55	115.92	122.96
2	E	400	ZGA	OBF-CBV-CBQ	-3.50	99.84	103.98
2	F	400	ZGA	OBD-CBH-CAQ	3.45	119.21	111.38
2	C	400	ZGA	OBC-CBG-CAC	3.44	117.41	111.09
2	F	400	ZGA	OBF-CBV-CBQ	-3.27	100.11	103.98
2	C	400	ZGA	OBD-CBH-CAQ	3.23	118.72	111.38
2	B	400	ZGA	OBC-CBG-CAC	3.18	116.94	111.09
2	D	400	ZGA	OBC-CBG-CAC	3.08	116.76	111.09
2	C	400	ZGA	OBC-CBG-OAG	-3.06	116.89	122.96
2	E	400	ZGA	OBC-CBG-OAG	-3.00	117.01	122.96
2	E	400	ZGA	OBD-CBH-CAQ	2.96	118.10	111.38
2	D	400	ZGA	CBB-CBN-CAR	-2.72	104.97	110.92
2	D	400	ZGA	OBF-CBV-CBQ	-2.70	100.78	103.98
2	D	400	ZGA	CAR-CAQ-CBH	2.51	128.25	122.62
2	F	400	ZGA	OBF-CBW-CBT	-2.49	99.94	103.58
2	A	400	ZGA	CAD-CBN-CAR	-2.43	105.49	110.86
2	C	400	ZGA	CAR-CAQ-CBH	-2.43	117.17	122.62
2	D	400	ZGA	CBR-OBC-CBG	2.24	120.51	116.68
2	B	400	ZGA	OBC-CBG-OAG	-2.24	118.52	122.96
2	F	400	ZGA	CAF-CBP-CBA	2.22	113.30	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	ZGA	OBF-CBW-CBT	-2.17	100.41	103.58
2	F	400	ZGA	OBC-CBG-OAG	-2.12	118.75	122.96
2	B	400	ZGA	OBF-CBW-CBT	-2.10	100.52	103.58

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	400	ZGA	CBO-CBB-CBN-CAD
2	D	400	ZGA	CBO-CBB-CBN-CAR
2	F	400	ZGA	CBO-CBB-CBN-CAD
2	F	400	ZGA	CBO-CBB-CBN-CAR
2	F	400	ZGA	CBN-CBB-CBO-CAX
2	C	400	ZGA	CBN-CBB-CBO-CAX
2	D	400	ZGA	OAH-CBH-OB-DBT
2	F	400	ZGA	CAQ-CAR-CBN-CBB
2	B	400	ZGA	CAY-CAZ-CBV-OB
2	D	400	ZGA	CAQ-CBH-OB-DBT
2	C	400	ZGA	CBN-CBB-CBO-CAE
2	C	400	ZGA	CBO-CBB-CBN-CAD
2	C	400	ZGA	CBO-CBB-CBN-CAR
2	D	400	ZGA	CAR-CAQ-CBH-OB

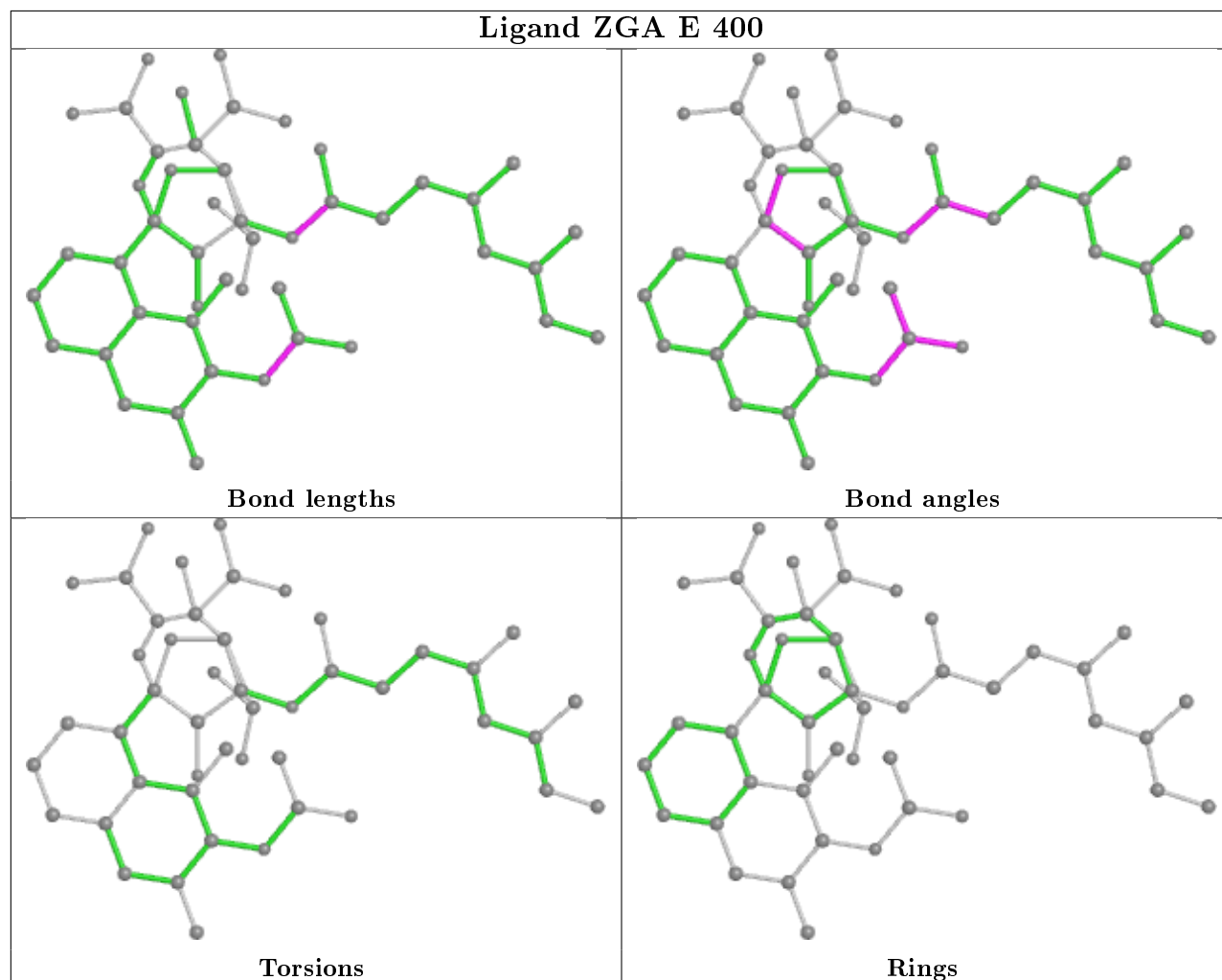
There are no ring outliers.

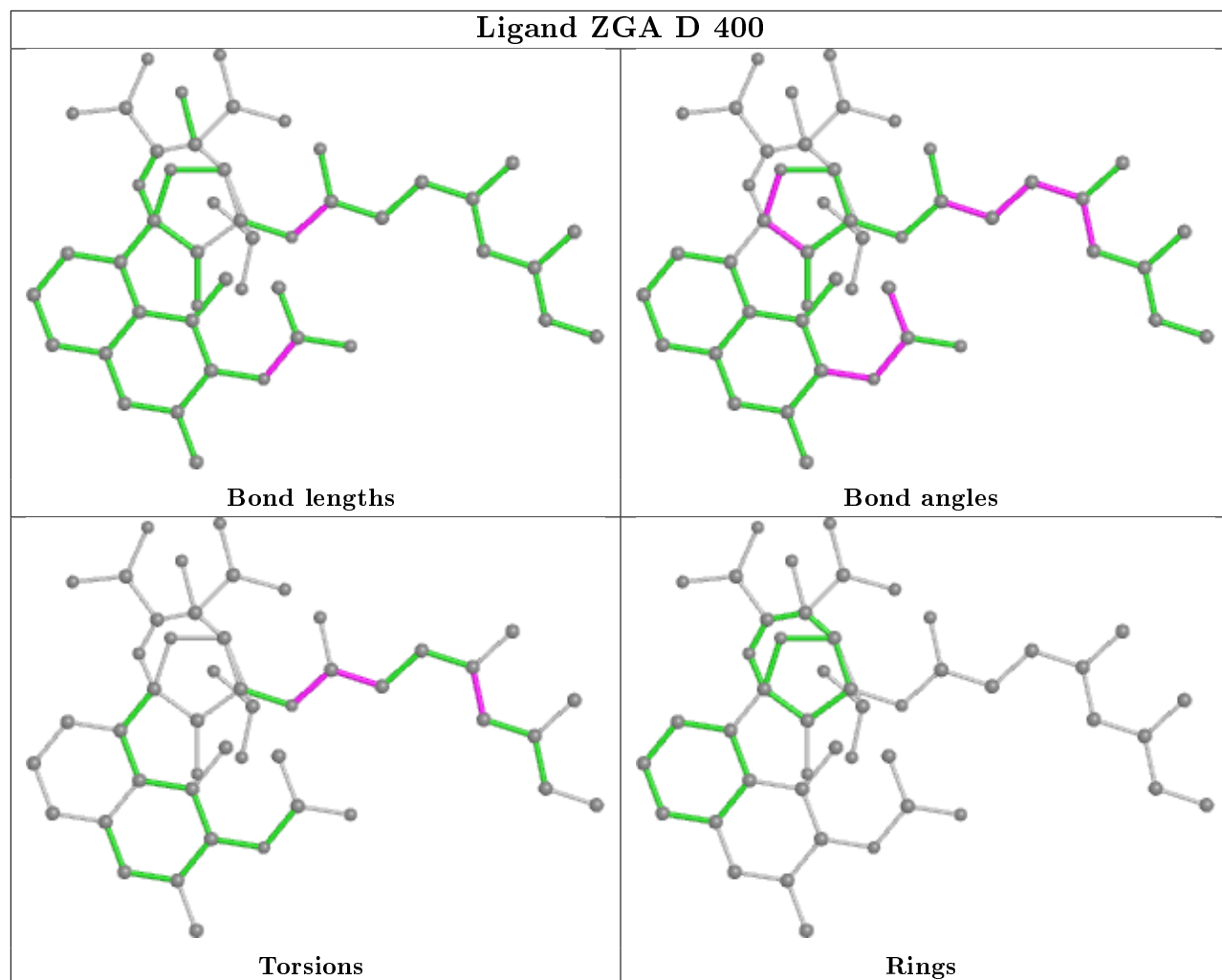
5 monomers are involved in 9 short contacts:

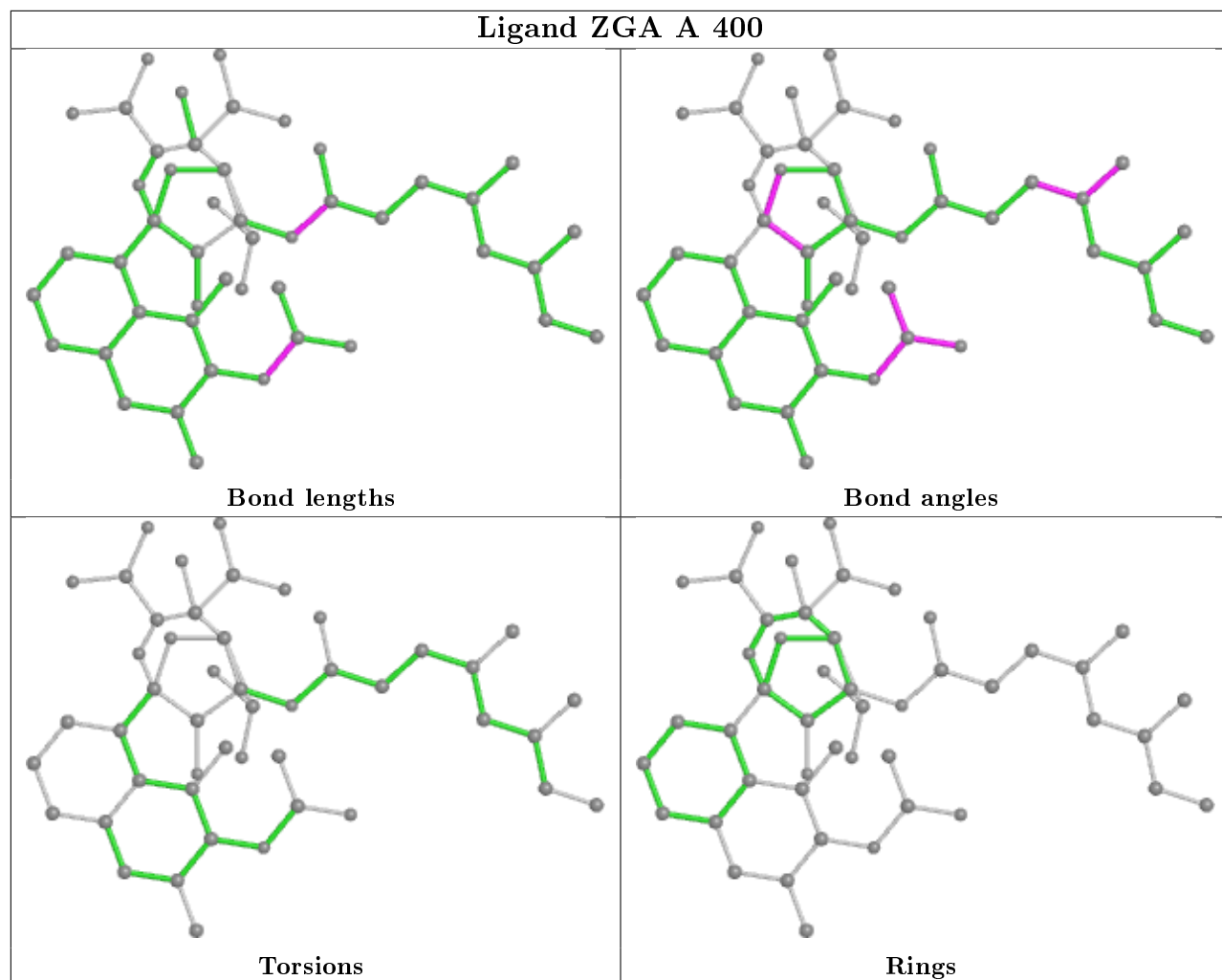
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	400	ZGA	1	0
2	D	400	ZGA	4	0
2	F	400	ZGA	2	0
2	C	400	ZGA	1	0
3	D	401	PO4	1	0

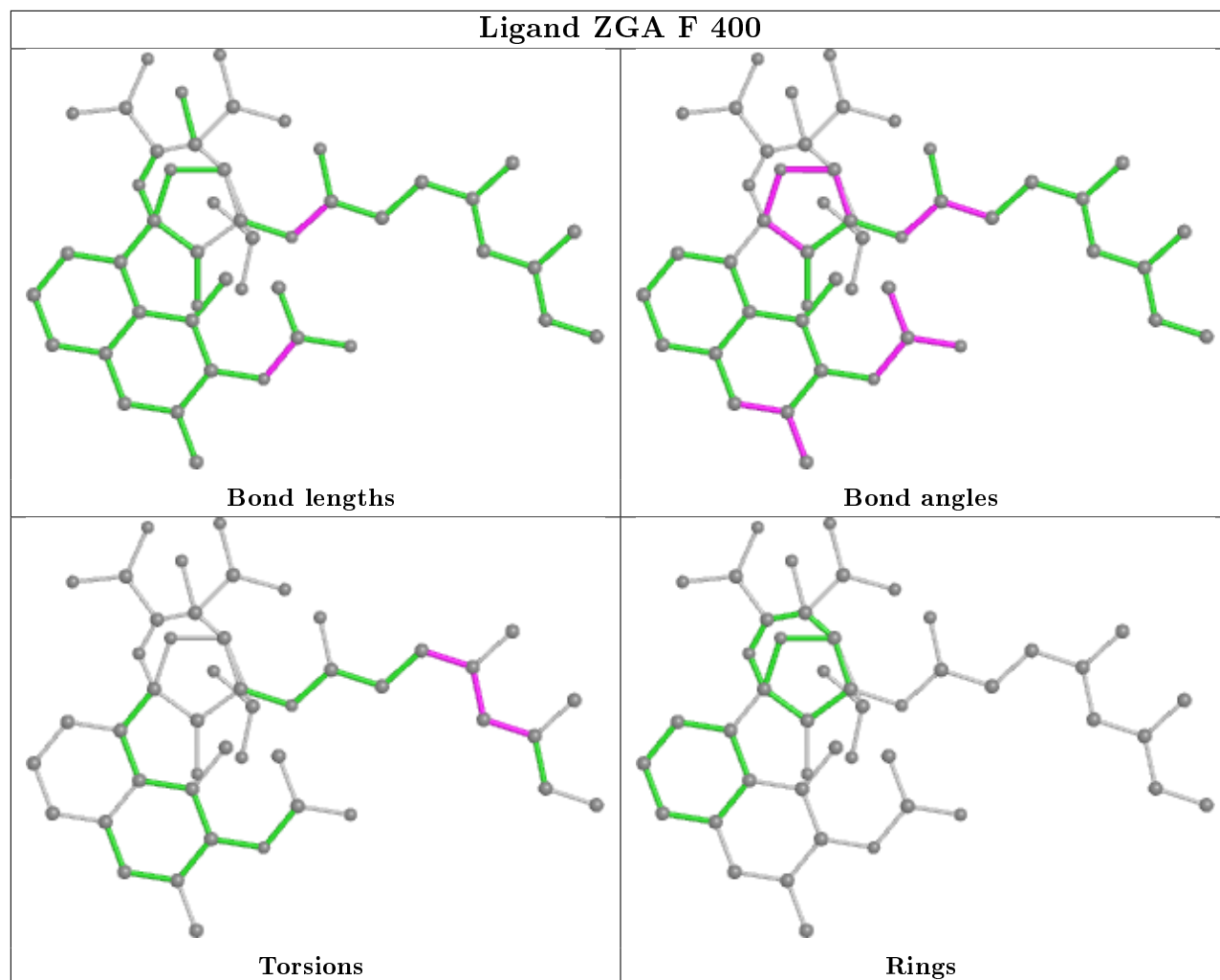
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

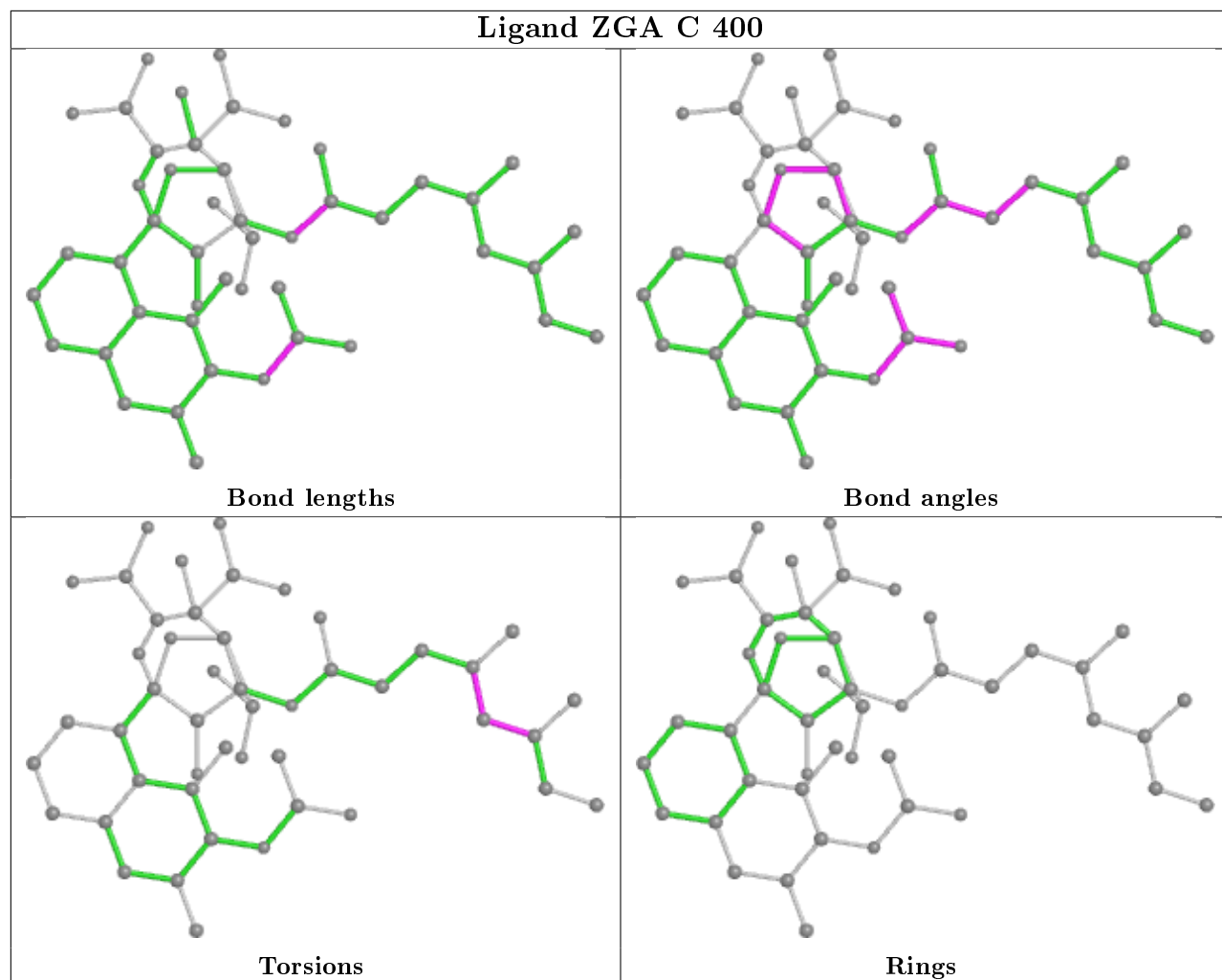
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

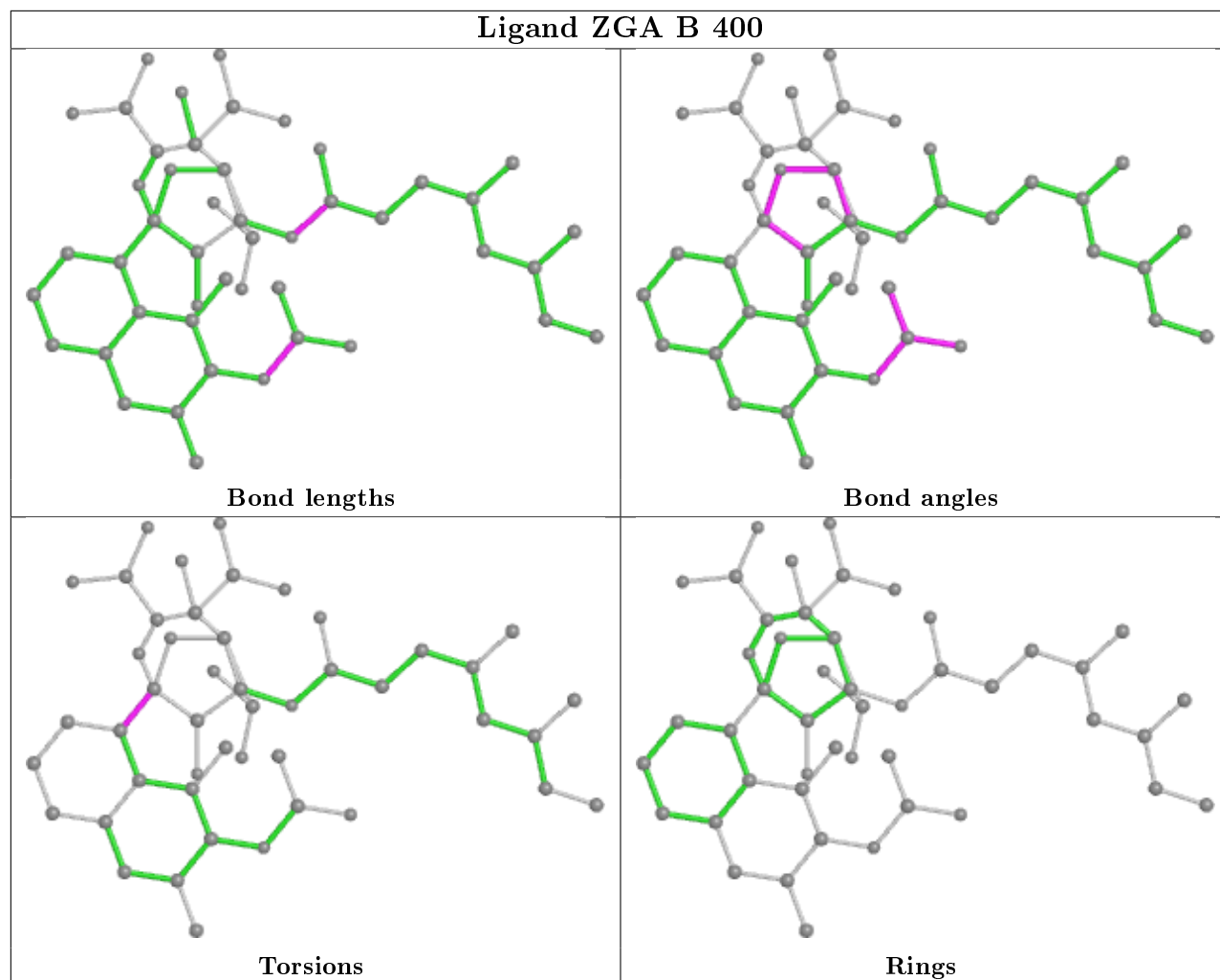












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/343 (97%)	-0.07	15 (4%) 33 36	11, 19, 46, 76	0
1	B	333/343 (97%)	-0.07	12 (3%) 42 45	14, 23, 48, 69	0
1	C	332/343 (96%)	-0.02	11 (3%) 46 49	12, 21, 46, 72	0
1	D	333/343 (97%)	0.41	32 (9%) 8 9	22, 39, 87, 108	0
1	E	333/343 (97%)	0.33	37 (11%) 5 6	16, 35, 88, 100	0
1	F	332/343 (96%)	0.96	68 (20%) 1 1	22, 57, 113, 132	0
All	All	1997/2058 (97%)	0.25	175 (8%) 10 11	11, 30, 92, 132	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	318	LYS	8.4
1	E	318	LYS	7.7
1	D	316	ILE	7.6
1	F	313	ALA	7.2
1	F	241	LYS	7.1
1	D	319	GLY	7.0
1	A	318	LYS	6.4
1	D	318	LYS	6.2
1	F	159	ASP	6.1
1	C	315	LYS	6.0
1	F	315	LYS	6.0
1	E	313	ALA	5.9
1	B	313	ALA	5.8
1	E	159	ASP	5.6
1	B	318	LYS	5.5
1	D	317	ARG	5.4
1	F	87	THR	5.3
1	F	319	GLY	5.3
1	C	313	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	86	MET	5.1
1	C	318	LYS	5.0
1	F	316	ILE	5.0
1	F	321	ALA	5.0
1	A	313	ALA	4.9
1	F	312	GLY	4.8
1	D	313	ALA	4.6
1	F	115	LYS	4.6
1	F	119	ARG	4.5
1	F	320	GLN	4.5
1	A	317	ARG	4.4
1	E	312	GLY	4.3
1	E	321	ALA	4.3
1	D	91	GLU	4.3
1	E	314	VAL	4.3
1	E	241	LYS	4.2
1	D	159	ASP	4.2
1	F	314	VAL	4.2
1	D	90	VAL	4.2
1	F	117	LYS	4.2
1	E	319	GLY	4.2
1	F	242	LYS	4.2
1	F	324	LEU	4.1
1	A	319	GLY	4.1
1	E	320	GLN	4.0
1	F	114	SER	4.0
1	A	324	LEU	4.0
1	A	323	THR	3.9
1	D	37	SER	3.9
1	F	91	GLU	3.9
1	A	315	LYS	3.9
1	D	113	GLU	3.9
1	E	315	LYS	3.9
1	A	320	GLN	3.8
1	F	90	VAL	3.8
1	E	242	LYS	3.8
1	B	316	ILE	3.8
1	A	321	ALA	3.8
1	D	92	LYS	3.8
1	F	250	GLU	3.7
1	A	36	LEU	3.7
1	B	37	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	317	ARG	3.6
1	F	113	GLU	3.6
1	D	38	SER	3.6
1	C	351	ASP	3.6
1	E	369	GLN	3.5
1	E	324	LEU	3.5
1	C	316	ILE	3.5
1	D	312	GLY	3.5
1	D	315	LYS	3.5
1	E	316	ILE	3.5
1	F	166	GLN	3.5
1	F	317	ARG	3.4
1	F	221	LEU	3.4
1	E	88	ILE	3.4
1	F	100	PHE	3.4
1	C	159	ASP	3.3
1	B	225	GLN	3.3
1	D	117	LYS	3.3
1	E	347	HIS	3.3
1	E	351	ASP	3.2
1	F	236	TRP	3.2
1	F	157	PHE	3.2
1	D	115	LYS	3.2
1	E	323	THR	3.1
1	F	155	ALA	3.1
1	F	89	SER	3.1
1	E	87	THR	3.1
1	E	225	GLN	3.1
1	B	159	ASP	3.0
1	E	221	LEU	3.0
1	F	254	LEU	2.9
1	E	37	SER	2.9
1	C	317	ARG	2.9
1	A	322	VAL	2.9
1	C	319	GLY	2.9
1	D	76	LEU	2.9
1	A	312	GLY	2.9
1	E	91	GLU	2.9
1	F	158	LEU	2.9
1	F	249	PRO	2.8
1	F	311	LYS	2.8
1	E	226	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	69	VAL	2.8
1	E	115	LYS	2.7
1	B	319	GLY	2.7
1	F	107	PRO	2.7
1	E	352	SER	2.7
1	D	111	PHE	2.7
1	F	38	SER	2.7
1	E	228	ARG	2.7
1	E	86	MET	2.7
1	F	82	LEU	2.7
1	E	236	TRP	2.6
1	D	89	SER	2.6
1	C	312	GLY	2.6
1	F	256	VAL	2.6
1	B	241	LYS	2.6
1	A	159	ASP	2.6
1	D	137	GLU	2.6
1	D	119	ARG	2.6
1	F	228	ARG	2.6
1	F	99	ASN	2.5
1	D	324	LEU	2.5
1	F	243	LEU	2.5
1	D	179	VAL	2.5
1	F	92	LYS	2.4
1	F	120	GLN	2.4
1	F	233	GLN	2.4
1	D	108	ASP	2.4
1	D	347	HIS	2.4
1	F	170	LYS	2.4
1	F	137	GLU	2.4
1	F	322	VAL	2.4
1	F	200	ASP	2.4
1	E	117	LYS	2.4
1	F	84	ASP	2.4
1	A	314	VAL	2.4
1	C	314	VAL	2.4
1	F	156	GLU	2.4
1	E	243	LEU	2.3
1	F	246	PHE	2.3
1	E	224	GLN	2.3
1	F	76	LEU	2.3
1	F	310	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	52	ARG	2.3
1	F	79	LEU	2.3
1	B	315	LYS	2.3
1	F	252	ILE	2.3
1	D	103	PHE	2.3
1	F	161	HIS	2.3
1	D	104	LEU	2.3
1	E	222	GLU	2.3
1	F	112	MET	2.2
1	B	314	VAL	2.2
1	F	240	VAL	2.2
1	F	369	GLN	2.2
1	E	248	LYS	2.2
1	F	248	LYS	2.2
1	D	130	LEU	2.2
1	F	116	GLU	2.2
1	A	316	ILE	2.2
1	F	88	ILE	2.2
1	D	361	GLN	2.2
1	E	166	GLN	2.2
1	F	103	PHE	2.2
1	B	249	PRO	2.1
1	B	250	GLU	2.1
1	D	107	PRO	2.1
1	D	75	VAL	2.1
1	F	108	ASP	2.1
1	F	72	PHE	2.0
1	E	247	ALA	2.0
1	D	166	GLN	2.0
1	C	241	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands

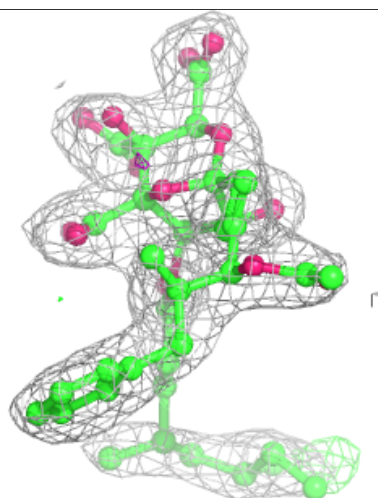
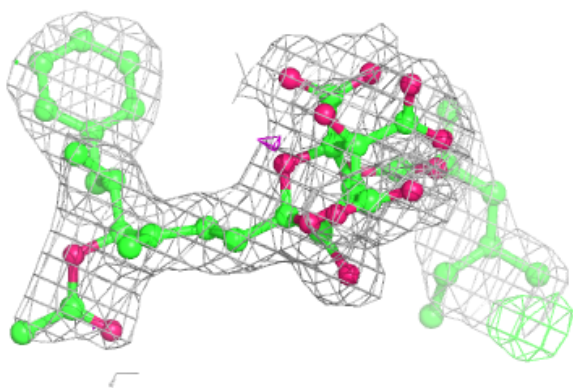
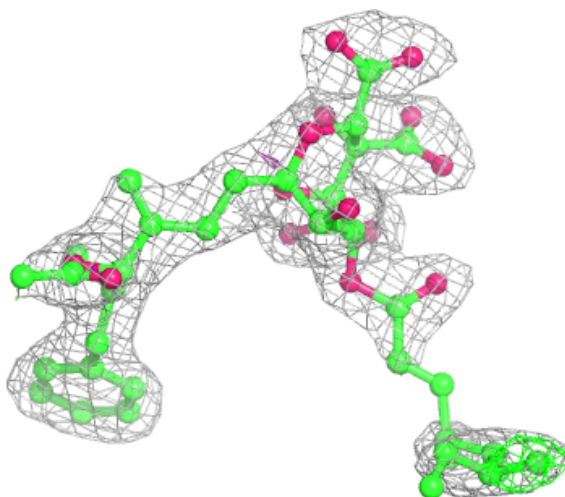
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZGA	F	400	49/49	0.88	0.17	43,52,61,63	0
2	ZGA	D	400	49/49	0.91	0.14	32,42,56,57	0
2	ZGA	E	400	49/49	0.93	0.11	23,35,47,50	0
2	ZGA	B	400	49/49	0.94	0.10	19,25,38,40	0
2	ZGA	C	400	49/49	0.95	0.10	15,23,37,39	0
2	ZGA	A	400	49/49	0.95	0.09	14,23,31,33	0
3	PO4	F	401	5/5	0.96	0.16	69,70,71,72	0
3	PO4	E	401	5/5	0.99	0.05	27,28,31,32	0
3	PO4	D	401	5/5	0.99	0.08	48,50,50,51	0
4	MG	B	402	1/1	0.99	0.05	32,32,32,32	0
4	MG	D	402	1/1	0.99	0.07	42,42,42,42	0
3	PO4	A	401	5/5	0.99	0.05	20,20,21,22	0
3	PO4	B	401	5/5	0.99	0.05	22,23,24,24	0
3	PO4	C	401	5/5	1.00	0.05	18,20,23,23	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.

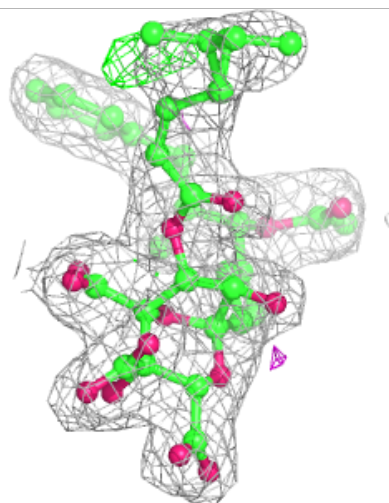
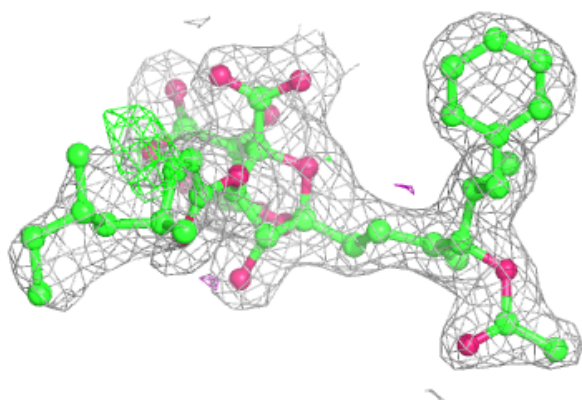
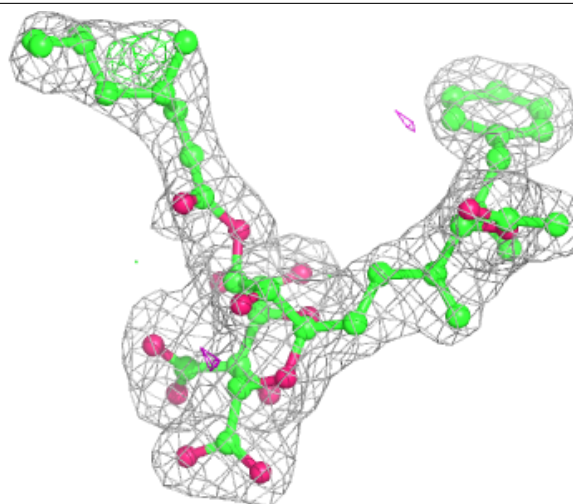
Electron density around ZGA F 400:

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



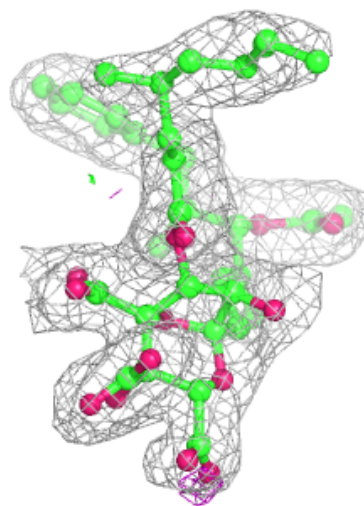
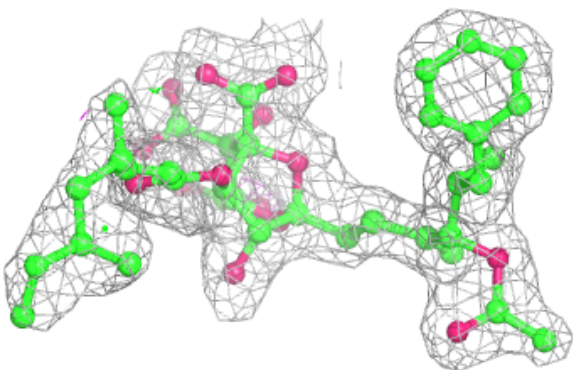
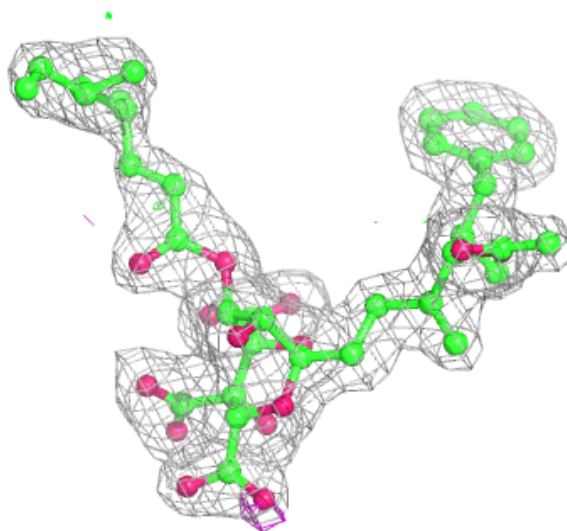
Electron density around ZGA D 400:

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



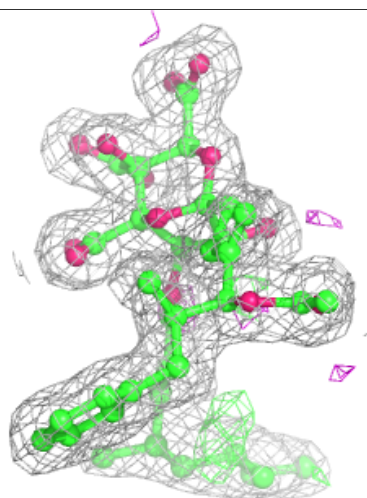
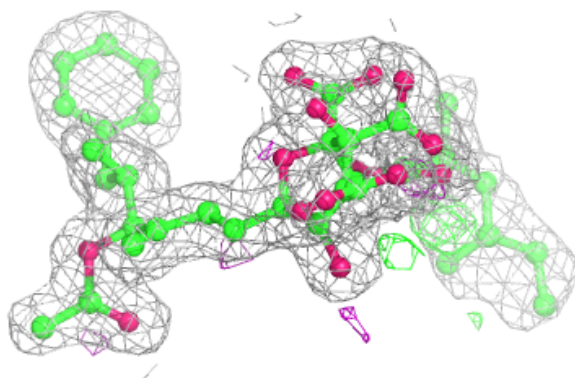
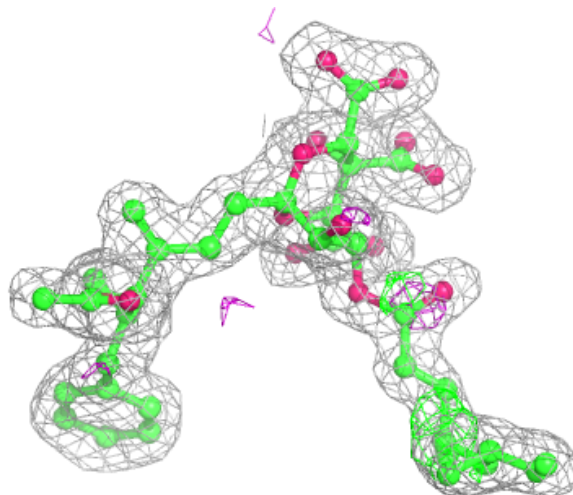
Electron density around ZGA E 400:

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



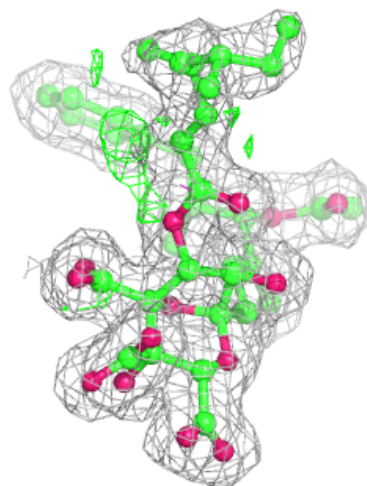
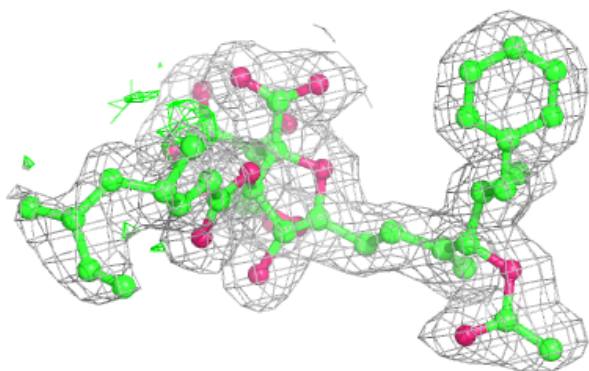
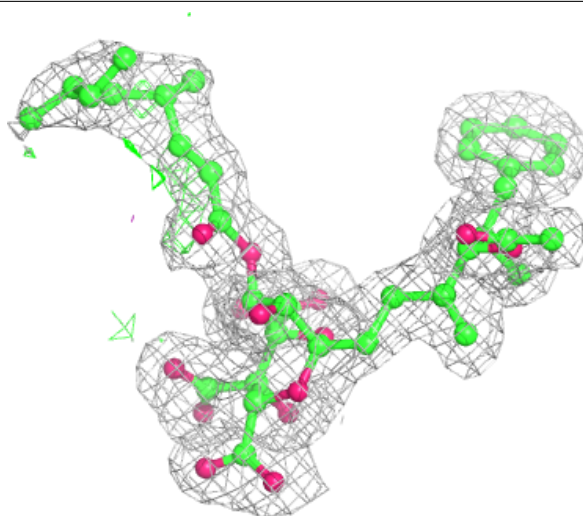
Electron density around ZGA B 400:

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



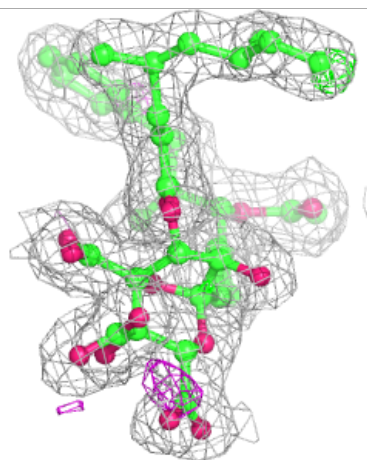
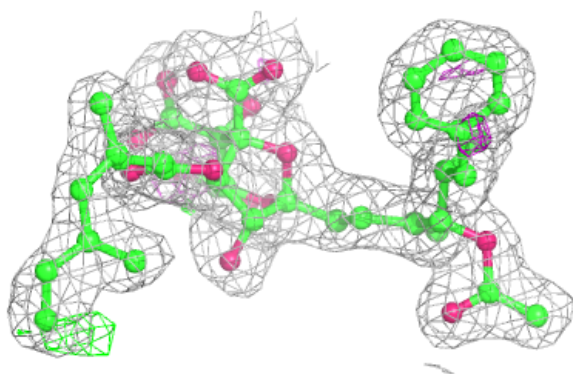
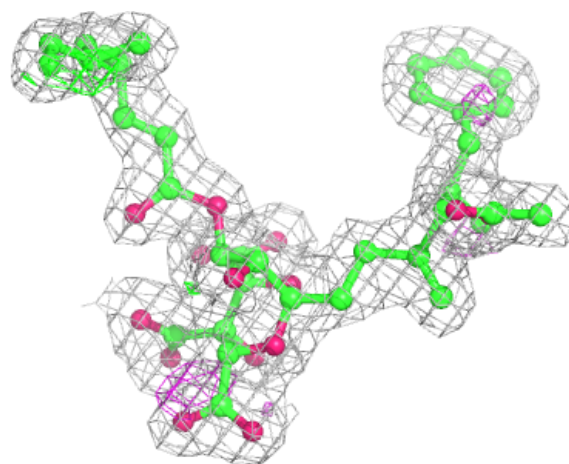
Electron density around ZGA C 400:

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



Electron density around ZGA A 400:

$2mF_o-DF_c$ (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.