



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:14 AM UTC

PDB ID : 3ED1 / pdb_00003ed1
Title : Crystal Structure of Rice GID1 complexed with GA3
Authors : Shimada, A.; Nakatsu, T.; Ueguchi-Tanaka, M.; Kato, H.; Matsuoka, M.
Deposited on : 2008-09-02
Resolution : 1.90 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

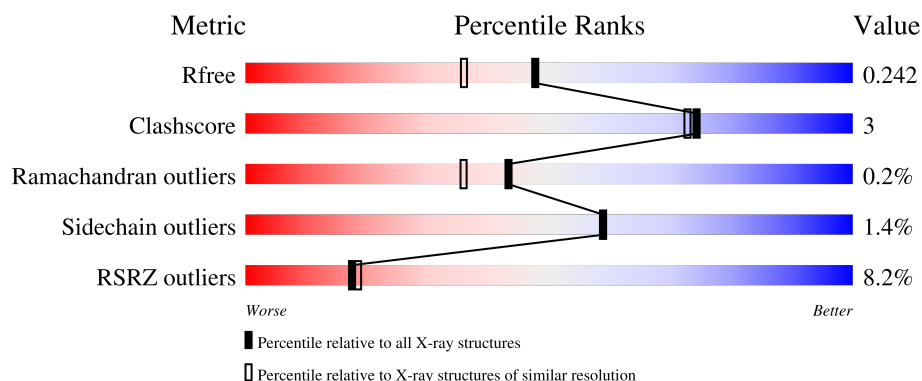
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	365	2% 80% 7% 12%
1	B	365	5% 82% 5% 13%
1	C	365	4% 73% 9% 18%
1	D	365	7% 79% 7% 14%
1	E	365	18% 78% 7% 14%

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Mol	Chain	Length	Quality of chain
1	F	365	5% 79% 5% 16%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15936 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 Gibberellin receptor GID1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	4	0
			2510	1591	447	462	10			
1	B	316	Total	C	N	O	S	0	5	0
			2476	1572	441	453	10			
1	C	301	Total	C	N	O	S	0	3	0
			2365	1507	416	432	10			
1	D	315	Total	C	N	O	S	0	3	0
			2455	1561	429	455	10			
1	E	313	Total	C	N	O	S	0	2	0
			2390	1526	416	437	11			
1	F	305	Total	C	N	O	S	0	2	0
			2378	1518	416	434	10			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLY	-	expression tag	UNP Q6L545
A	356	SER	-	expression tag	UNP Q6L545
A	357	HIS	-	expression tag	UNP Q6L545
A	358	HIS	-	expression tag	UNP Q6L545
A	359	HIS	-	expression tag	UNP Q6L545
A	360	HIS	-	expression tag	UNP Q6L545
A	361	HIS	-	expression tag	UNP Q6L545
A	362	HIS	-	expression tag	UNP Q6L545
A	363	HIS	-	expression tag	UNP Q6L545
A	364	HIS	-	expression tag	UNP Q6L545
A	365	HIS	-	expression tag	UNP Q6L545
A	366	HIS	-	expression tag	UNP Q6L545
B	355	GLY	-	expression tag	UNP Q6L545
B	356	SER	-	expression tag	UNP Q6L545
B	357	HIS	-	expression tag	UNP Q6L545
B	358	HIS	-	expression tag	UNP Q6L545
B	359	HIS	-	expression tag	UNP Q6L545

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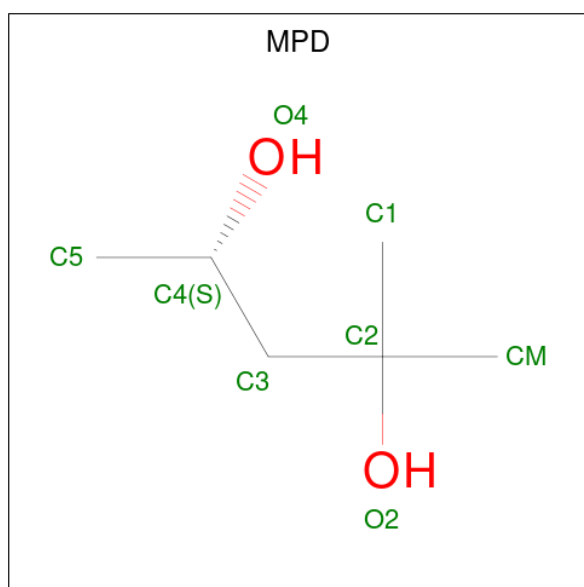
Chain	Residue	Modelled	Actual	Comment	Reference
B	360	HIS	-	expression tag	UNP Q6L545
B	361	HIS	-	expression tag	UNP Q6L545
B	362	HIS	-	expression tag	UNP Q6L545
B	363	HIS	-	expression tag	UNP Q6L545
B	364	HIS	-	expression tag	UNP Q6L545
B	365	HIS	-	expression tag	UNP Q6L545
B	366	HIS	-	expression tag	UNP Q6L545
C	355	GLY	-	expression tag	UNP Q6L545
C	356	SER	-	expression tag	UNP Q6L545
C	357	HIS	-	expression tag	UNP Q6L545
C	358	HIS	-	expression tag	UNP Q6L545
C	359	HIS	-	expression tag	UNP Q6L545
C	360	HIS	-	expression tag	UNP Q6L545
C	361	HIS	-	expression tag	UNP Q6L545
C	362	HIS	-	expression tag	UNP Q6L545
C	363	HIS	-	expression tag	UNP Q6L545
C	364	HIS	-	expression tag	UNP Q6L545
C	365	HIS	-	expression tag	UNP Q6L545
C	366	HIS	-	expression tag	UNP Q6L545
D	355	GLY	-	expression tag	UNP Q6L545
D	356	SER	-	expression tag	UNP Q6L545
D	357	HIS	-	expression tag	UNP Q6L545
D	358	HIS	-	expression tag	UNP Q6L545
D	359	HIS	-	expression tag	UNP Q6L545
D	360	HIS	-	expression tag	UNP Q6L545
D	361	HIS	-	expression tag	UNP Q6L545
D	362	HIS	-	expression tag	UNP Q6L545
D	363	HIS	-	expression tag	UNP Q6L545
D	364	HIS	-	expression tag	UNP Q6L545
D	365	HIS	-	expression tag	UNP Q6L545
D	366	HIS	-	expression tag	UNP Q6L545
E	355	GLY	-	expression tag	UNP Q6L545
E	356	SER	-	expression tag	UNP Q6L545
E	357	HIS	-	expression tag	UNP Q6L545
E	358	HIS	-	expression tag	UNP Q6L545
E	359	HIS	-	expression tag	UNP Q6L545
E	360	HIS	-	expression tag	UNP Q6L545
E	361	HIS	-	expression tag	UNP Q6L545
E	362	HIS	-	expression tag	UNP Q6L545
E	363	HIS	-	expression tag	UNP Q6L545
E	364	HIS	-	expression tag	UNP Q6L545
E	365	HIS	-	expression tag	UNP Q6L545

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Chain	Residue	Modelled	Actual	Comment	Reference
E	366	HIS	-	expression tag	UNP Q6L545
F	355	GLY	-	expression tag	UNP Q6L545
F	356	SER	-	expression tag	UNP Q6L545
F	357	HIS	-	expression tag	UNP Q6L545
F	358	HIS	-	expression tag	UNP Q6L545
F	359	HIS	-	expression tag	UNP Q6L545
F	360	HIS	-	expression tag	UNP Q6L545
F	361	HIS	-	expression tag	UNP Q6L545
F	362	HIS	-	expression tag	UNP Q6L545
F	363	HIS	-	expression tag	UNP Q6L545
F	364	HIS	-	expression tag	UNP Q6L545
F	365	HIS	-	expression tag	UNP Q6L545
F	366	HIS	-	expression tag	UNP Q6L545

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



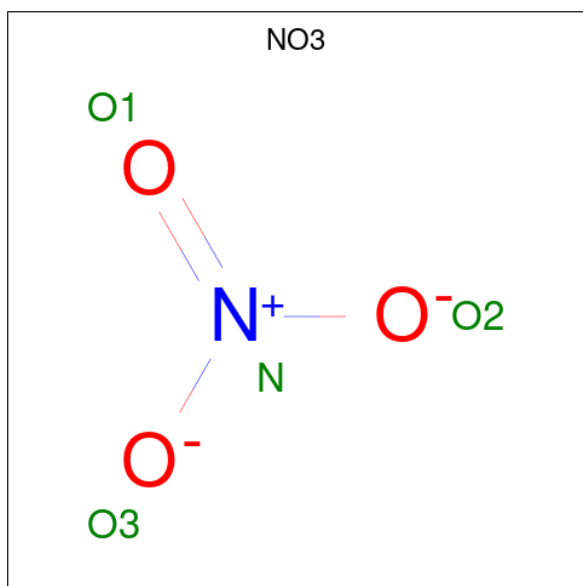
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



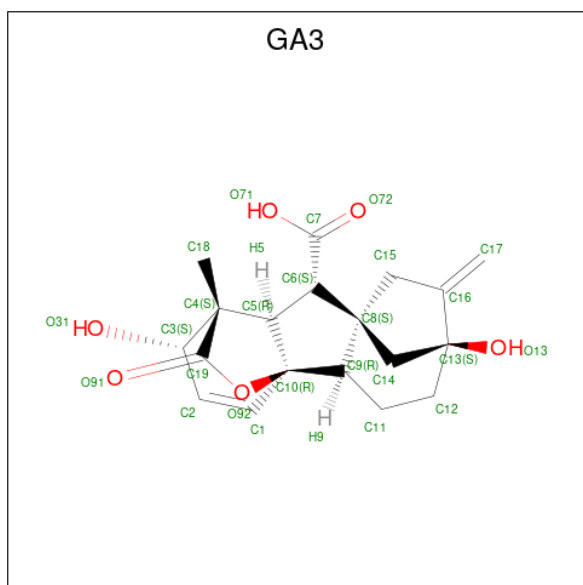
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	B	1	Total	N	O	0	0
			4	1	3		
3	B	1	Total	N	O	0	0
			4	1	3		
3	B	1	Total	N	O	0	0
			4	1	3		
3	C	1	Total	N	O	0	0
			4	1	3		
3	C	1	Total	N	O	0	0
			4	1	3		
3	D	1	Total	N	O	0	0
			4	1	3		
3	D	1	Total	N	O	0	0
			4	1	3		

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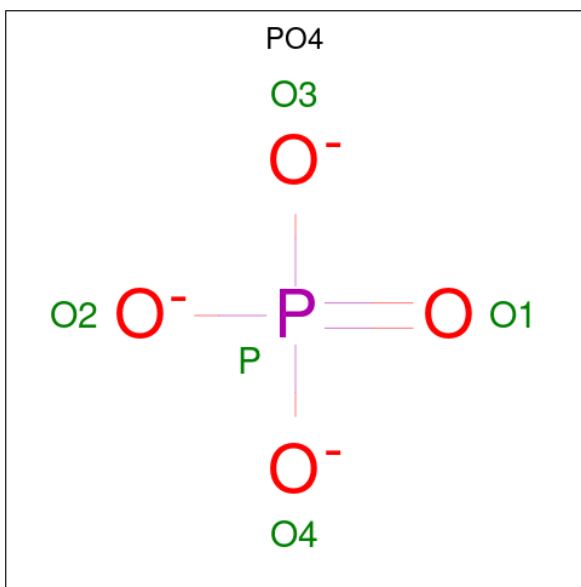
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	N	O	0	0
			4	1	3		
3	F	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is GIBBERELLIN A3 (CCD ID: GA3) (formula: $C_{19}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			25	19	6		
4	B	1	Total	C	O	0	0
			25	19	6		
4	C	1	Total	C	O	0	0
			25	19	6		
4	D	1	Total	C	O	0	0
			25	19	6		
4	E	1	Total	C	O	0	0
			25	19	6		
4	F	1	Total	C	O	0	0
			25	19	6		

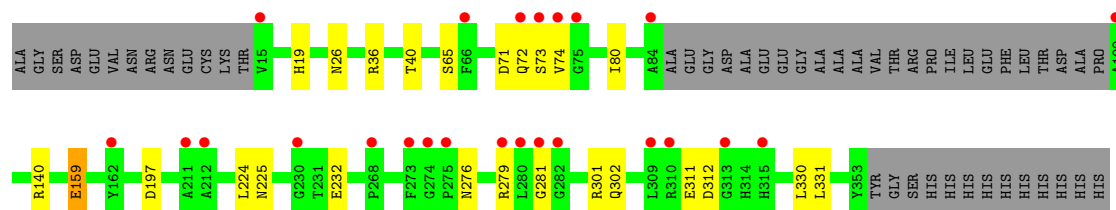
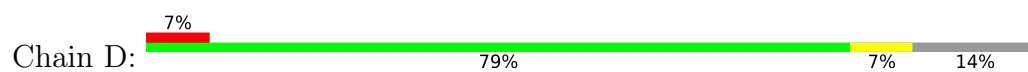
- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



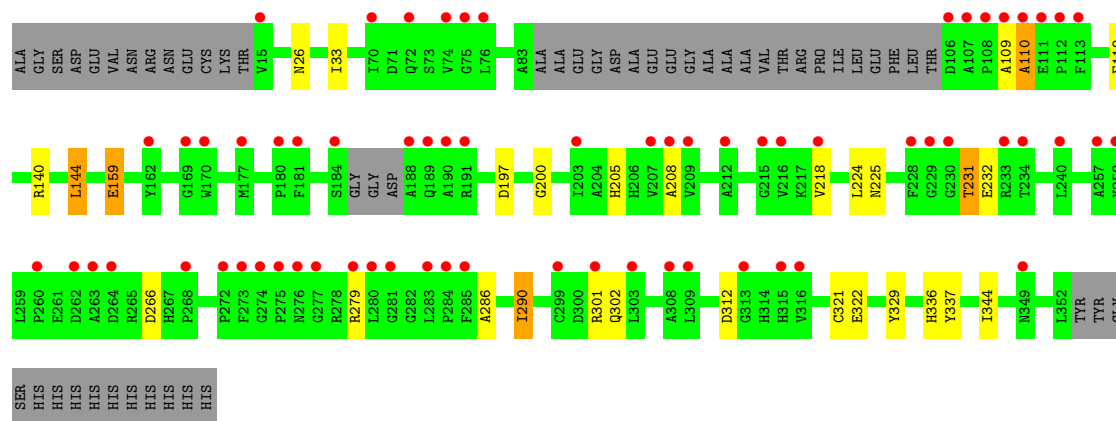
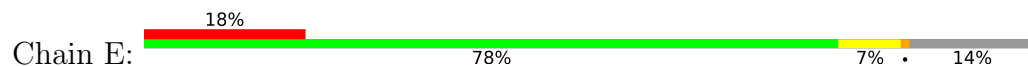
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

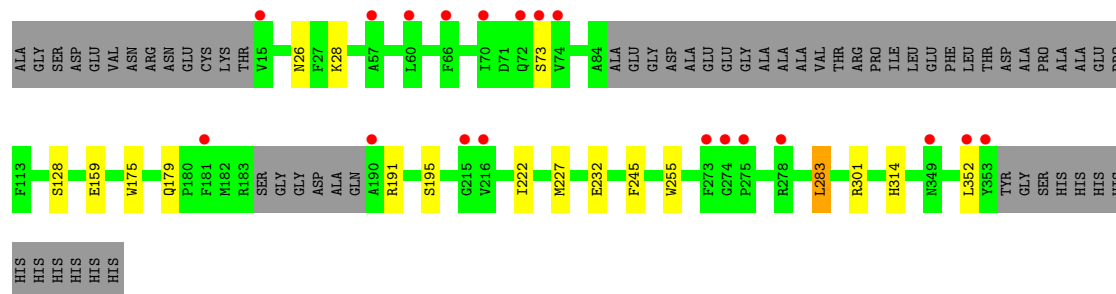
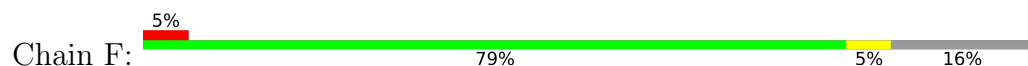
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	239	Total	O	0	0
			239	239		
6	B	193	Total	O	0	0
			193	193		
6	C	173	Total	O	0	0
			173	173		
6	D	204	Total	O	0	0
			204	204		
6	E	123	Total	O	0	0
			123	123		
6	F	174	Total	O	0	0
			174	174		



• Molecule 1: Gibberellin receptor GID1



• Molecule 1: Gibberellin receptor GID1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.72Å 134.14Å 118.87Å 90.00° 105.20° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.90) 97.5 (20.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.239 0.199 , 0.242	Depositor DCC
R_{free} test set	9653 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15936	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: NO3, MPD, PO4, GA3

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	0/2593	0.88	2/3524 (0.1%)
1	B	0.81	0/2561	0.88	0/3480
1	C	0.77	0/2440	0.92	3/3313 (0.1%)
1	D	0.81	0/2533	0.90	0/3446
1	E	0.70	0/2461	0.90	0/3352
1	F	0.75	0/2449	0.88	0/3328
All	All	0.78	0/15037	0.89	5/20443 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	274	GLY	CA-C-N	6.42	127.87	119.84
1	C	274	GLY	C-N-CA	6.42	127.87	119.84
1	C	192	VAL	N-CA-C	6.12	117.11	108.36
1	A	30[A]	SER	N-CA-C	-5.20	105.53	111.14
1	A	30[B]	SER	N-CA-C	-5.20	105.53	111.14

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	2510	0	2387	16	0
1	B	2476	0	2367	12	0
1	C	2365	0	2245	19	0
1	D	2455	0	2315	15	0
1	E	2390	0	2242	19	0
1	F	2378	0	2246	8	0
2	A	8	0	14	1	0
2	B	8	0	14	2	0
2	C	8	0	14	0	0
2	D	8	0	14	0	0
2	E	8	0	14	1	0
2	F	8	0	14	1	0
3	A	12	0	0	1	0
3	B	12	0	0	1	0
3	C	8	0	0	2	0
3	D	8	0	0	0	0
3	F	8	0	0	0	0
4	A	25	0	21	0	0
4	B	25	0	21	0	0
4	C	25	0	21	0	0
4	D	25	0	21	0	0
4	E	25	0	21	0	0
4	F	25	0	21	0	0
5	B	5	0	0	0	0
5	E	5	0	0	0	0
6	A	239	0	0	0	0
6	B	193	0	0	1	0
6	C	173	0	0	1	0
6	D	204	0	0	1	0
6	E	123	0	0	0	0
6	F	174	0	0	0	0
All	All	15936	0	14012	88	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 3.

All (88) 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:26:ASN:HD22	1:B:26:ASN:HD22	1.29	0.81
1:A:15:VAL:HG12	1:A:16:VAL:H	1.52	0.73
2:E:501:MPD:H13	2:F:501:MPD:H13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:ILE:HG13	1:E:290:ILE:O	1.93	0.67
1:C:177:MET:HE3	1:C:216:VAL:CG1	2.28	0.64
1:A:177:MET:HE3	1:A:216:VAL:HG13	1.78	0.64
1:A:28[A]:LYS:HE3	1:A:245:PHE:O	1.98	0.63
1:D:279:ARG:HD2	1:D:312:ASP:OD2	1.99	0.63
1:C:347:PHE:O	1:C:351:ASN:ND2	2.33	0.62
1:F:232:GLU:O	1:F:301:ARG:NH2	2.34	0.60
1:E:109:ALA:O	1:E:110:ALA:HB3	2.02	0.59
1:C:26:ASN:HD22	1:D:26:ASN:HD22	1.49	0.58
1:B:175:TRP:O	1:B:179:GLN:HG2	2.03	0.57
1:A:231:THR:HG22	3:A:602:NO3:O3	2.06	0.56
1:C:231:THR:HG22	3:C:602:NO3:O2	2.05	0.56
1:D:279:ARG:HH12	1:D:311:GLU:HB2	1.70	0.55
1:F:283:LEU:O	1:F:314:HIS:HE1	1.90	0.55
1:E:144:LEU:HD11	1:E:344:ILE:HG22	1.89	0.55
1:C:232:GLU:O	1:C:301:ARG:NH2	2.41	0.54
2:A:501:MPD:HM2	2:B:501:MPD:H13	1.90	0.53
1:E:26:ASN:HD22	1:F:26:ASN:HD22	1.57	0.53
1:E:232:GLU:O	1:E:301:ARG:NH2	2.42	0.53
1:D:330:LEU:O	1:D:331:LEU:HD23	2.09	0.53
1:F:227:MET:HG2	1:F:255:TRP:CZ2	2.44	0.52
1:E:159:GLU:H	1:E:159:GLU:CD	2.18	0.52
1:C:144:LEU:C	1:C:144:LEU:HD12	2.35	0.52
1:B:301:ARG:HH11	1:B:301:ARG:HG2	1.75	0.51
1:D:232:GLU:O	1:D:301:ARG:NH2	2.43	0.51
1:A:177:MET:CE	1:A:216:VAL:CG1	2.89	0.51
1:F:191:ARG:NH1	1:F:352:LEU:O	2.44	0.51
1:C:173:LEU:HD11	1:C:177:MET:HE2	1.93	0.50
1:A:287:LYS:HD2	1:A:351:ASN:OD1	2.11	0.50
1:A:177:MET:HE3	1:A:216:VAL:CG1	2.42	0.50
1:B:213:ASP:CG	1:B:278:ARG:HH22	2.20	0.49
1:D:279:ARG:HH12	1:D:311:GLU:CB	2.24	0.49
1:A:227:MET:HG2	1:A:255:TRP:CZ2	2.48	0.48
1:E:205:HIS:O	1:E:208:ALA:HB3	2.13	0.48
1:D:65:SER:HA	1:D:80:ILE:O	2.13	0.48
1:A:30[A]:SER:OG	3:B:604:NO3:O1	2.27	0.48
1:E:119:PHE:O	1:E:200:GLY:HA3	2.14	0.48
1:E:140:ARG:HD3	1:E:337:TYR:OH	2.14	0.47
1:E:144:LEU:HD12	1:E:144:LEU:C	2.40	0.47
1:B:232:GLU:O	1:B:301:ARG:NH2	2.48	0.47
1:E:218:VAL:HB	1:E:286:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:ASN:HA	1:E:302:GLN:OE1	2.14	0.46
1:D:140:ARG:NH1	6:D:787:HOH:O	2.47	0.46
1:C:223:LEU:HB3	1:C:226:ALA:HB2	1.97	0.46
1:C:65:SER:HA	1:C:80:ILE:O	2.16	0.46
1:B:227:MET:HG2	1:B:255:TRP:CZ2	2.51	0.46
1:C:71:ASP:HB3	1:C:76:LEU:HB3	1.99	0.45
1:D:36:ARG:HD2	1:D:40:THR:OG1	2.17	0.45
1:D:71:ASP:C	1:D:73:SER:H	2.24	0.45
1:B:157:ALA:HB1	1:B:158:PRO:HA	1.99	0.45
1:B:26:ASN:HB3	2:B:501:MPD:HM2	1.99	0.44
1:C:157:ALA:HB1	1:C:158:PRO:HA	1.98	0.44
1:E:109:ALA:O	1:E:110:ALA:CB	2.63	0.44
1:A:232:GLU:O	1:A:301:ARG:NH2	2.50	0.44
1:A:157:ALA:HB1	1:A:158:PRO:HA	2.00	0.44
1:A:321:CYS:HB3	1:A:336:HIS:CG	2.53	0.44
1:D:159:GLU:H	1:D:159:GLU:HG2	1.14	0.43
1:A:210:ARG:O	1:A:214:GLU:HG3	2.19	0.43
1:F:175:TRP:O	1:F:179:GLN:HG2	2.18	0.43
1:D:281:GLY:HA2	1:D:312:ASP:O	2.18	0.43
1:E:279:ARG:HD2	1:E:312:ASP:OD2	2.19	0.43
1:C:197:ASP:HA	1:C:224:LEU:O	2.19	0.43
1:C:74:VAL:HG12	1:C:76:LEU:HB2	2.00	0.43
1:A:197:ASP:HA	1:A:224:LEU:O	2.19	0.43
1:C:177:MET:HE3	1:C:216:VAL:HG13	2.01	0.43
1:B:213:ASP:OD1	1:B:278:ARG:NH2	2.51	0.42
1:B:287:LYS:HG2	1:B:315:HIS:HB3	2.01	0.42
1:B:238[A]:ARG:NH2	6:B:854:HOH:O	2.52	0.42
1:C:179:GLN:HA	1:C:180:PRO:HD3	1.97	0.41
1:C:310:ARG:NH1	6:C:628:HOH:O	2.52	0.41
1:E:197:ASP:HA	1:E:224:LEU:O	2.19	0.41
1:B:35:ARG:HD3	1:B:254:TYR:CZ	2.56	0.41
1:A:173:LEU:O	1:A:177:MET:HG2	2.20	0.41
1:C:28[A]:LYS:HE3	1:C:245:PHE:O	2.21	0.41
1:C:119:PHE:O	1:C:200:GLY:HA3	2.20	0.41
1:D:197:ASP:HA	1:D:224:LEU:O	2.20	0.41
1:E:231:THR:OG1	1:E:266:ASP:OD1	2.35	0.41
1:F:195:SER:HA	1:F:222:ILE:O	2.21	0.40
3:C:604:NO3:O3	1:D:19:HIS:NE2	2.50	0.40
1:D:225:ASN:HA	1:D:302:GLN:OE1	2.21	0.40
1:C:227:MET:HG2	1:C:255:TRP:CZ2	2.56	0.40
1:F:28[A]:LYS:HE3	1:F:245:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:ASP:OD2	1:E:329:TYR:OH	2.37	0.40
1:E:321:CYS:HB3	1:E:336:HIS:CG	2.57	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	321/365 (88%)	310 (97%)	11 (3%)	0	100	100
1	B	315/365 (86%)	303 (96%)	12 (4%)	0	100	100
1	C	298/365 (82%)	288 (97%)	10 (3%)	0	100	100
1	D	314/365 (86%)	305 (97%)	8 (2%)	1 (0%)	36	29
1	E	309/365 (85%)	297 (96%)	11 (4%)	1 (0%)	36	29
1	F	301/365 (82%)	291 (97%)	9 (3%)	1 (0%)	36	29
All	All	1858/2190 (85%)	1794 (97%)	61 (3%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	72	GLN
1	E	110	ALA
1	F	73	SER

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	260/302 (86%)	256 (98%)	4 (2%)	57	56
1	B	258/302 (85%)	256 (99%)	2 (1%)	73	75
1	C	244/302 (81%)	240 (98%)	4 (2%)	55	54
1	D	251/302 (83%)	248 (99%)	3 (1%)	63	63
1	E	239/302 (79%)	234 (98%)	5 (2%)	47	44
1	F	241/302 (80%)	238 (99%)	3 (1%)	63	63
All	All	1493/1812 (82%)	1472 (99%)	21 (1%)	59	59

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ILE
1	A	69	ILE
1	A	128	SER
1	A	261	GLU
1	B	53	VAL
1	B	249	GLN
1	C	33	ILE
1	C	74	VAL
1	C	128	SER
1	C	144	LEU
1	D	74	VAL
1	D	159	GLU
1	D	276	ASN
1	E	144	LEU
1	E	159	GLU
1	E	231	THR
1	E	290	ILE
1	E	322	GLU
1	F	128	SER
1	F	159	GLU
1	F	283	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	221	ASN

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Mol	Chain	Res	Type
1	B	26	ASN
1	B	160	HIS
1	C	26	ASN
1	C	206	HIS
1	C	221	ASN
1	D	68	HIS
1	D	221	ASN
1	E	68	HIS
1	E	206	HIS
1	E	221	ASN
1	F	19	HIS
1	F	26	ASN
1	F	179	GLN
1	F	221	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](#)

26 ligands are modelled in this entry.

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	NO3	B	601	-	1,3,3	3.54	1 (100%)	0,3,3	-	-
2	MPD	F	501	-	7,7,7	0.26	0	9,10,10	0.52	0
3	NO3	D	601	-	1,3,3	3.45	1 (100%)	0,3,3	-	-
4	GA3	A	401	-	28,29,29	1.18	2 (7%)	47,52,52	1.96	15 (31%)
3	NO3	A	603	-	1,3,3	3.31	1 (100%)	0,3,3	-	-
3	NO3	B	602	-	1,3,3	3.26	1 (100%)	0,3,3	-	-
4	GA3	E	401	-	28,29,29	1.41	3 (10%)	47,52,52	1.86	13 (27%)
2	MPD	D	501	-	7,7,7	0.49	0	9,10,10	0.39	0
2	MPD	C	501	-	7,7,7	0.39	0	9,10,10	0.49	0
3	NO3	B	604	-	1,3,3	3.29	1 (100%)	0,3,3	-	-
2	MPD	B	501	-	7,7,7	0.35	0	9,10,10	0.45	0
2	MPD	A	501	-	7,7,7	0.44	0	9,10,10	0.60	0
4	GA3	F	401	-	28,29,29	1.28	3 (10%)	47,52,52	1.72	11 (23%)
3	NO3	F	602	-	1,3,3	3.26	1 (100%)	0,3,3	-	-
3	NO3	F	603	-	1,3,3	3.26	1 (100%)	0,3,3	-	-
4	GA3	D	401	-	28,29,29	1.36	4 (14%)	47,52,52	1.74	6 (12%)
5	PO4	E	701	-	4,4,4	0.92	0	6,6,6	0.53	0
3	NO3	A	601	-	1,3,3	3.14	1 (100%)	0,3,3	-	-
4	GA3	B	401	-	28,29,29	1.51	3 (10%)	47,52,52	1.81	13 (27%)
3	NO3	A	602	-	1,3,3	3.59	1 (100%)	0,3,3	-	-
3	NO3	D	603	-	1,3,3	3.30	1 (100%)	0,3,3	-	-
4	GA3	C	401	-	28,29,29	1.20	2 (7%)	47,52,52	2.12	15 (31%)
3	NO3	C	602	-	1,3,3	3.28	1 (100%)	0,3,3	-	-
5	PO4	B	701	-	4,4,4	0.90	0	6,6,6	0.49	0
3	NO3	C	604	-	1,3,3	3.13	1 (100%)	0,3,3	-	-
2	MPD	E	501	-	7,7,7	0.30	0	9,10,10	0.37	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
2	MPD	F	501	-	-	0/5/5/5	-
2	MPD	D	501	-	-	0/5/5/5	-
2	MPD	C	501	-	-	0/5/5/5	-
4	GA3	A	401	-	-	0/4/84/84	-
4	GA3	B	401	-	-	0/4/84/84	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	B	501	-	-	0/5/5/5	-
2	MPD	A	501	-	-	0/5/5/5	-
4	GA3	F	401	-	-	0/4/84/84	-
2	MPD	E	501	-	-	0/5/5/5	-
4	GA3	D	401	-	-	0/4/84/84	-
4	GA3	C	401	-	-	0/4/84/84	-
4	GA3	E	401	-	-	0/4/84/84	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	GA3	O92-C19	5.03	1.46	1.36
4	E	401	GA3	O92-C19	4.85	1.45	1.36
4	F	401	GA3	O92-C19	4.50	1.44	1.36
4	D	401	GA3	O92-C19	4.12	1.44	1.36
3	A	602	NO3	O1-N	3.59	1.42	1.24
3	B	601	NO3	O1-N	3.54	1.41	1.24
4	C	401	GA3	O92-C19	3.50	1.43	1.36
3	D	601	NO3	O1-N	3.45	1.41	1.24
3	A	603	NO3	O1-N	3.31	1.40	1.24
3	D	603	NO3	O1-N	3.30	1.40	1.24
3	B	604	NO3	O1-N	3.29	1.40	1.24
4	D	401	GA3	O92-C10	-3.28	1.41	1.48
3	C	602	NO3	O1-N	3.28	1.40	1.24
3	F	603	NO3	O1-N	3.26	1.40	1.24
3	B	602	NO3	O1-N	3.26	1.40	1.24
3	F	602	NO3	O1-N	3.26	1.40	1.24
4	A	401	GA3	O92-C19	3.19	1.42	1.36
3	A	601	NO3	O1-N	3.14	1.39	1.24
3	C	604	NO3	O1-N	3.13	1.39	1.24
4	B	401	GA3	C3-C2	3.08	1.55	1.49
4	B	401	GA3	O92-C10	-2.96	1.42	1.48
4	E	401	GA3	O92-C10	-2.91	1.42	1.48
4	E	401	GA3	O71-C7	-2.31	1.23	1.30
4	D	401	GA3	C3-C2	2.13	1.53	1.49
4	A	401	GA3	O92-C10	-2.10	1.44	1.48
4	D	401	GA3	O71-C7	-2.04	1.24	1.30
4	F	401	GA3	O92-C10	-2.03	1.44	1.48
4	C	401	GA3	C13-C16	-2.02	1.50	1.52
4	F	401	GA3	C2-C1	2.01	1.35	1.32

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	GA3	C15-C16-C13	7.81	113.72	107.59
4	D	401	GA3	C15-C16-C13	6.82	112.95	107.59
4	B	401	GA3	C15-C16-C13	6.72	112.87	107.59
4	A	401	GA3	C15-C16-C13	6.51	112.70	107.59
4	F	401	GA3	C15-C16-C13	6.21	112.47	107.59
4	D	401	GA3	C14-C13-C16	-6.21	98.30	102.00
4	C	401	GA3	C14-C13-C16	-6.11	98.36	102.00
4	E	401	GA3	C15-C16-C13	5.96	112.27	107.59
4	A	401	GA3	C14-C13-C16	-4.87	99.09	102.00
4	E	401	GA3	C14-C8-C15	4.85	105.22	100.64
4	A	401	GA3	O13-C13-C16	-4.57	106.40	113.19
4	B	401	GA3	C14-C13-C16	-3.56	99.88	102.00
4	C	401	GA3	C9-C10-C1	-3.55	115.51	120.02
4	C	401	GA3	O92-C10-C9	3.54	113.96	110.14
4	F	401	GA3	C14-C13-C16	-3.54	99.89	102.00
4	E	401	GA3	C8-C6-C7	3.42	117.46	112.17
4	F	401	GA3	C15-C16-C17	-3.13	122.87	126.70
4	B	401	GA3	C8-C15-C16	-3.10	98.18	103.62
4	F	401	GA3	C8-C15-C16	-3.10	98.18	103.62
4	C	401	GA3	C15-C16-C17	-3.06	122.96	126.70
4	A	401	GA3	C9-C10-C1	-3.01	116.19	120.02
4	D	401	GA3	C15-C16-C17	-3.01	123.02	126.70
4	C	401	GA3	C8-C15-C16	-3.01	98.35	103.62
4	B	401	GA3	C14-C8-C15	2.86	103.34	100.64
4	A	401	GA3	C12-C13-C16	2.73	114.93	110.91
4	F	401	GA3	C10-O92-C19	-2.69	105.06	108.13
4	E	401	GA3	C18-C4-C3	2.69	114.55	110.47
4	C	401	GA3	O72-C7-C6	-2.68	116.76	123.37
4	E	401	GA3	C15-C8-C9	-2.65	105.51	109.86
4	C	401	GA3	C4-C5-C6	2.63	121.30	117.12
4	C	401	GA3	C11-C12-C13	-2.62	109.13	112.26
4	C	401	GA3	C8-C6-C7	2.62	116.22	112.17
4	F	401	GA3	O71-C7-C6	2.58	121.57	113.71
4	E	401	GA3	O71-C7-C6	2.57	121.56	113.71
4	A	401	GA3	C13-C16-C17	-2.56	122.81	125.16
4	A	401	GA3	C8-C15-C16	-2.55	99.15	103.62
4	A	401	GA3	O72-C7-C6	-2.54	117.11	123.37
4	A	401	GA3	C4-C5-C6	2.53	121.15	117.12
4	A	401	GA3	O71-C7-C6	2.52	121.40	113.71
4	E	401	GA3	C15-C16-C17	-2.52	123.62	126.70
4	F	401	GA3	C12-C13-C14	2.50	112.15	108.97
4	F	401	GA3	C11-C12-C13	-2.45	109.33	112.26
4	B	401	GA3	C15-C16-C17	-2.44	123.72	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	GA3	C14-C8-C15	2.39	102.89	100.64
4	C	401	GA3	C12-C13-C14	2.38	112.00	108.97
4	A	401	GA3	C18-C4-C3	2.36	114.05	110.47
4	E	401	GA3	C11-C12-C13	-2.35	109.45	112.26
4	A	401	GA3	C11-C12-C13	-2.35	109.45	112.26
4	B	401	GA3	C12-C13-C16	2.34	114.37	110.91
4	E	401	GA3	C11-C9-C8	-2.31	110.11	112.97
4	B	401	GA3	C9-C10-C1	-2.31	117.08	120.02
4	B	401	GA3	O31-C3-C2	-2.30	104.54	109.95
4	D	401	GA3	C8-C15-C16	-2.29	99.61	103.62
4	C	401	GA3	O71-C7-C6	2.26	120.59	113.71
4	E	401	GA3	O31-C3-C2	-2.25	104.67	109.95
4	B	401	GA3	C15-C8-C9	-2.24	106.18	109.86
4	E	401	GA3	C4-C5-C6	2.24	120.68	117.12
4	C	401	GA3	O31-C3-C2	-2.21	104.76	109.95
4	D	401	GA3	C12-C13-C16	2.20	114.16	110.91
4	A	401	GA3	O92-C10-C9	2.18	112.49	110.14
4	A	401	GA3	O13-C13-C12	2.15	112.64	108.00
4	F	401	GA3	C8-C6-C7	2.15	115.50	112.17
4	B	401	GA3	C18-C4-C3	2.14	113.72	110.47
4	F	401	GA3	O72-C7-C6	-2.10	118.19	123.37
4	B	401	GA3	O71-C7-C6	2.10	120.10	113.71
4	B	401	GA3	C11-C12-C13	-2.10	109.75	112.26
4	E	401	GA3	C12-C13-C14	-2.07	106.33	108.97
4	A	401	GA3	C8-C6-C7	2.05	115.34	112.17
4	D	401	GA3	C15-C8-C9	-2.03	106.53	109.86
4	C	401	GA3	C13-C16-C17	-2.01	123.32	125.16
4	E	401	GA3	C9-C10-C1	-2.01	117.47	120.02
4	B	401	GA3	O72-C7-C6	-2.00	118.44	123.37
4	F	401	GA3	C18-C4-C3	2.00	113.50	110.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 7 short contacts:

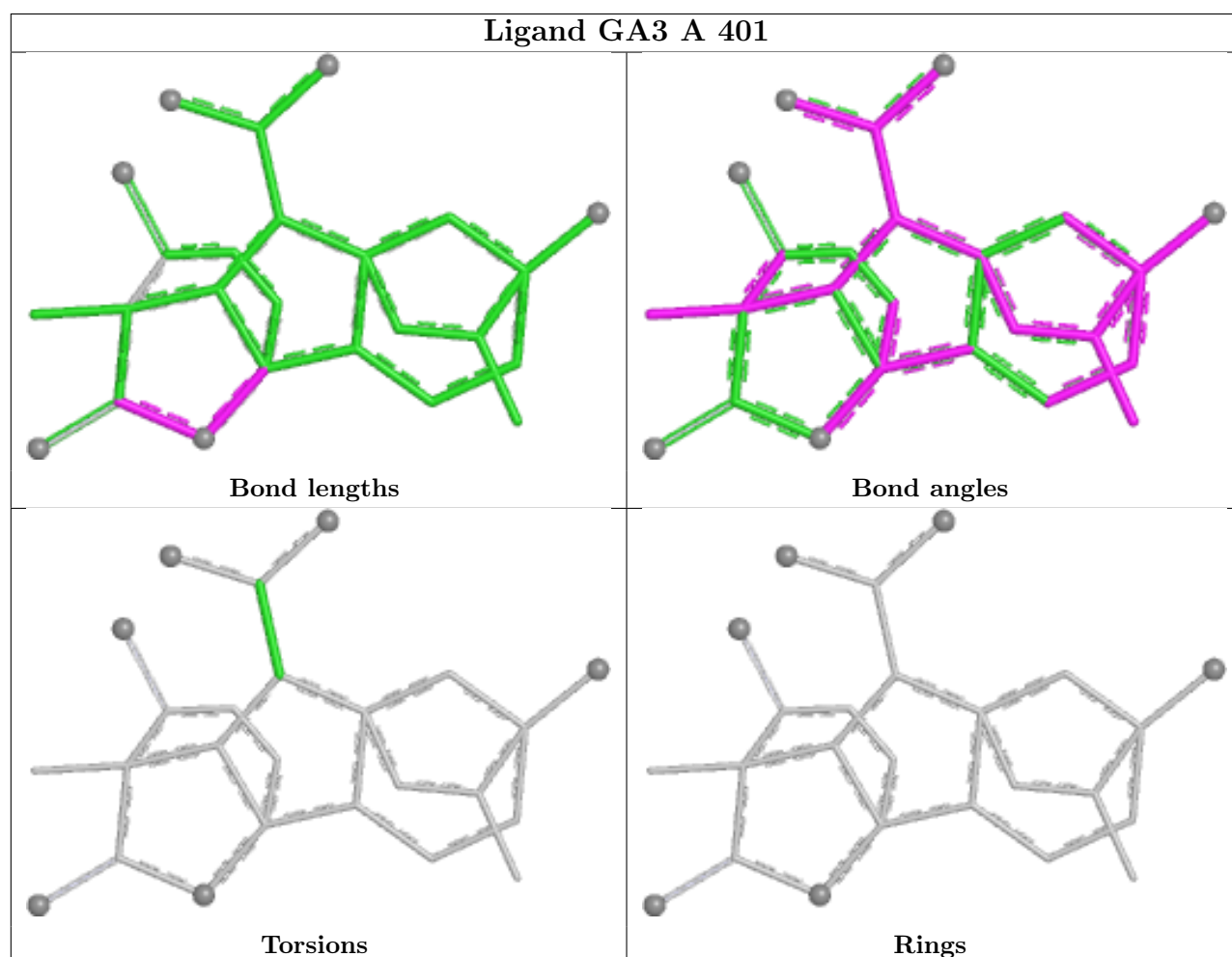
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	MPD	1	0
3	B	604	NO3	1	0
2	B	501	MPD	2	0
2	A	501	MPD	1	0

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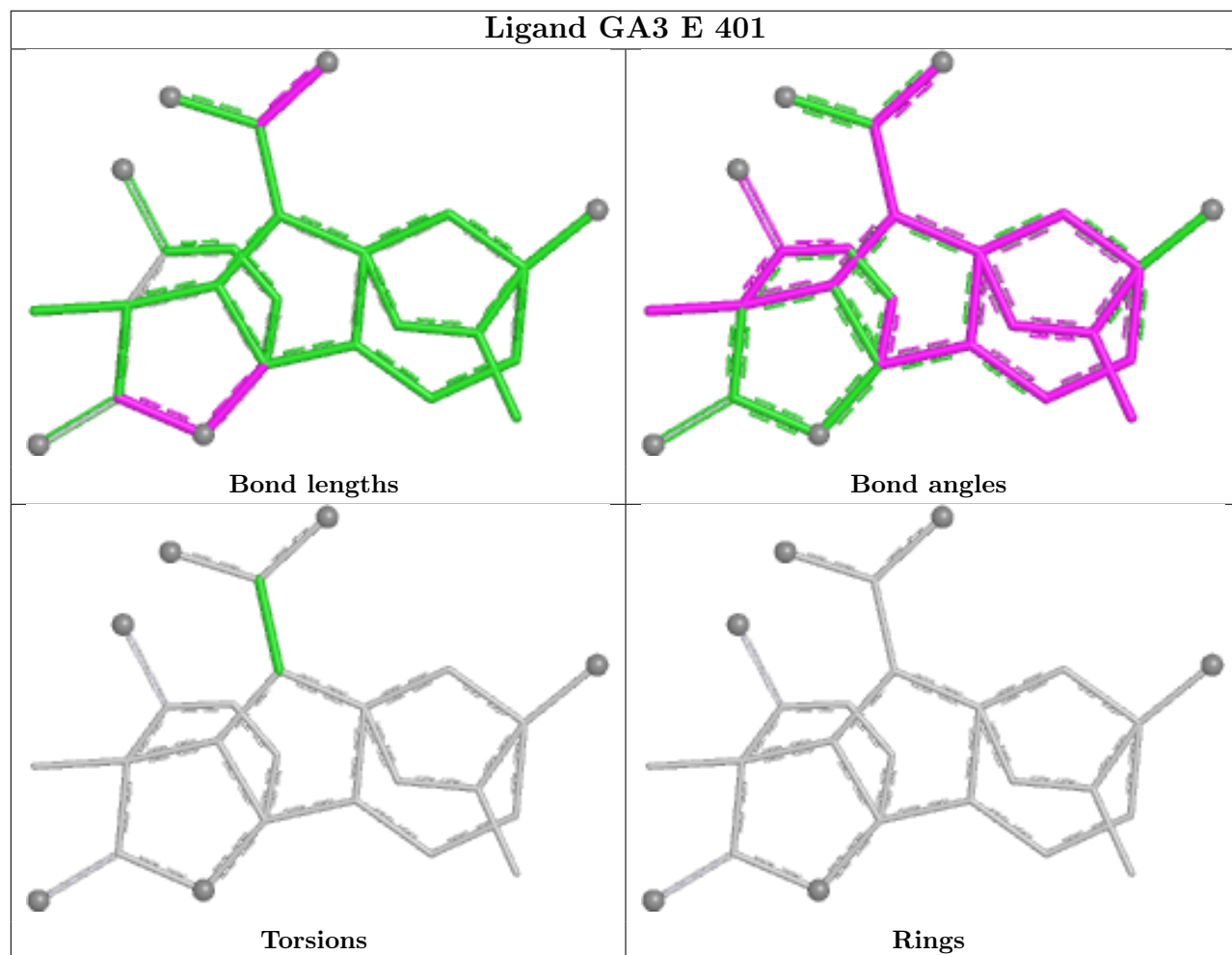
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	NO3	1	0
3	C	602	NO3	1	0
3	C	604	NO3	1	0
2	E	501	MPD	1	0

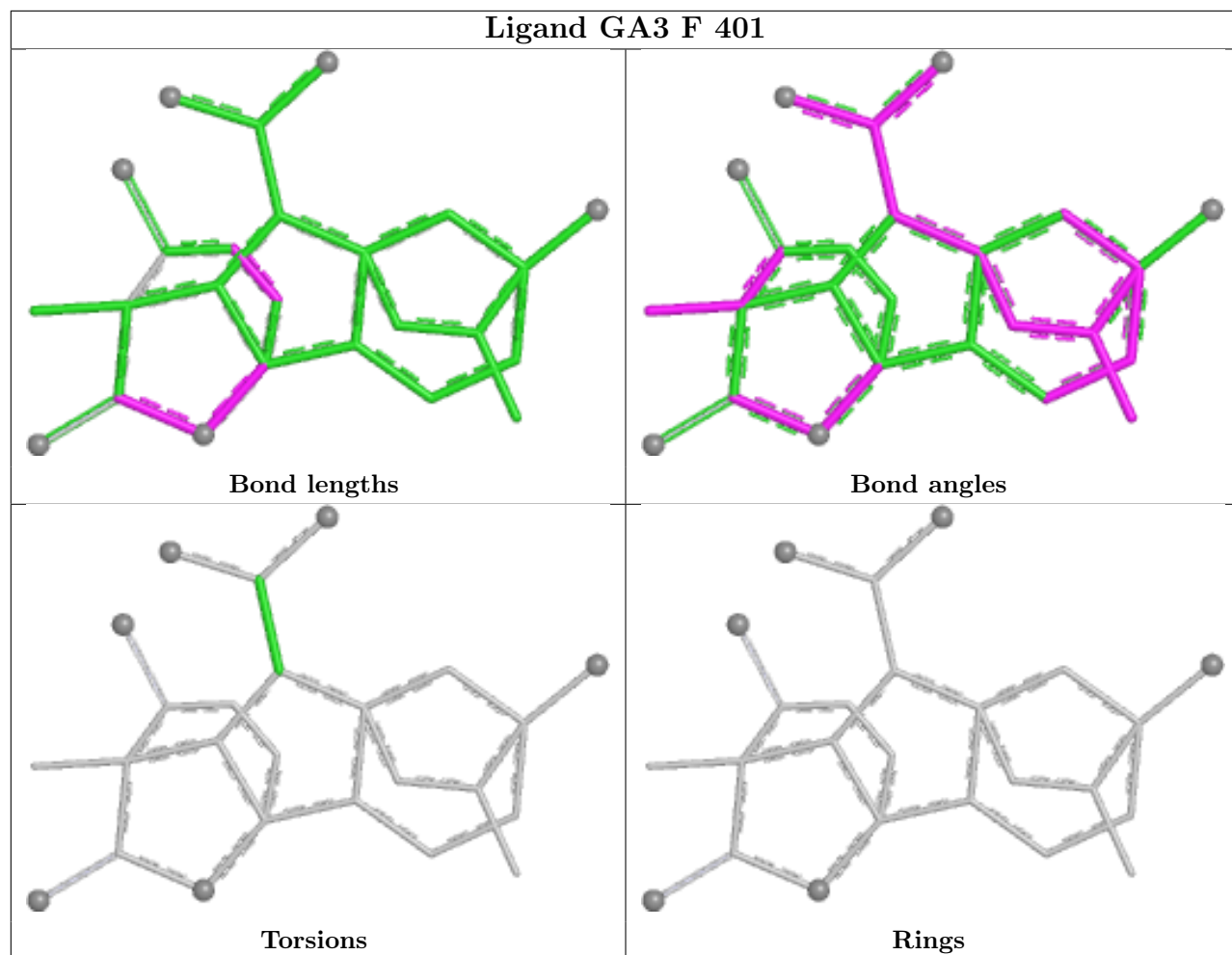
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



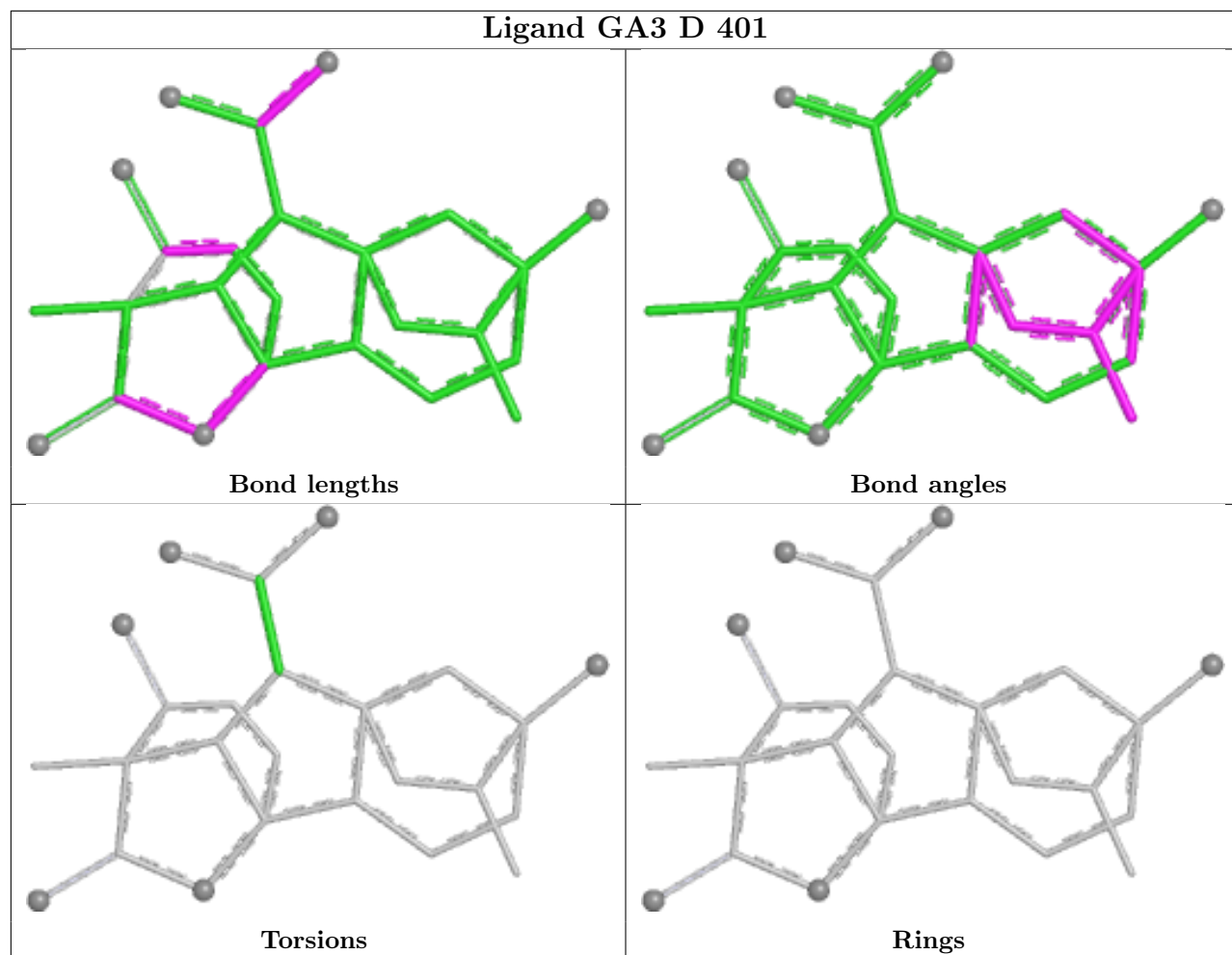
Ligand GA3 E 401



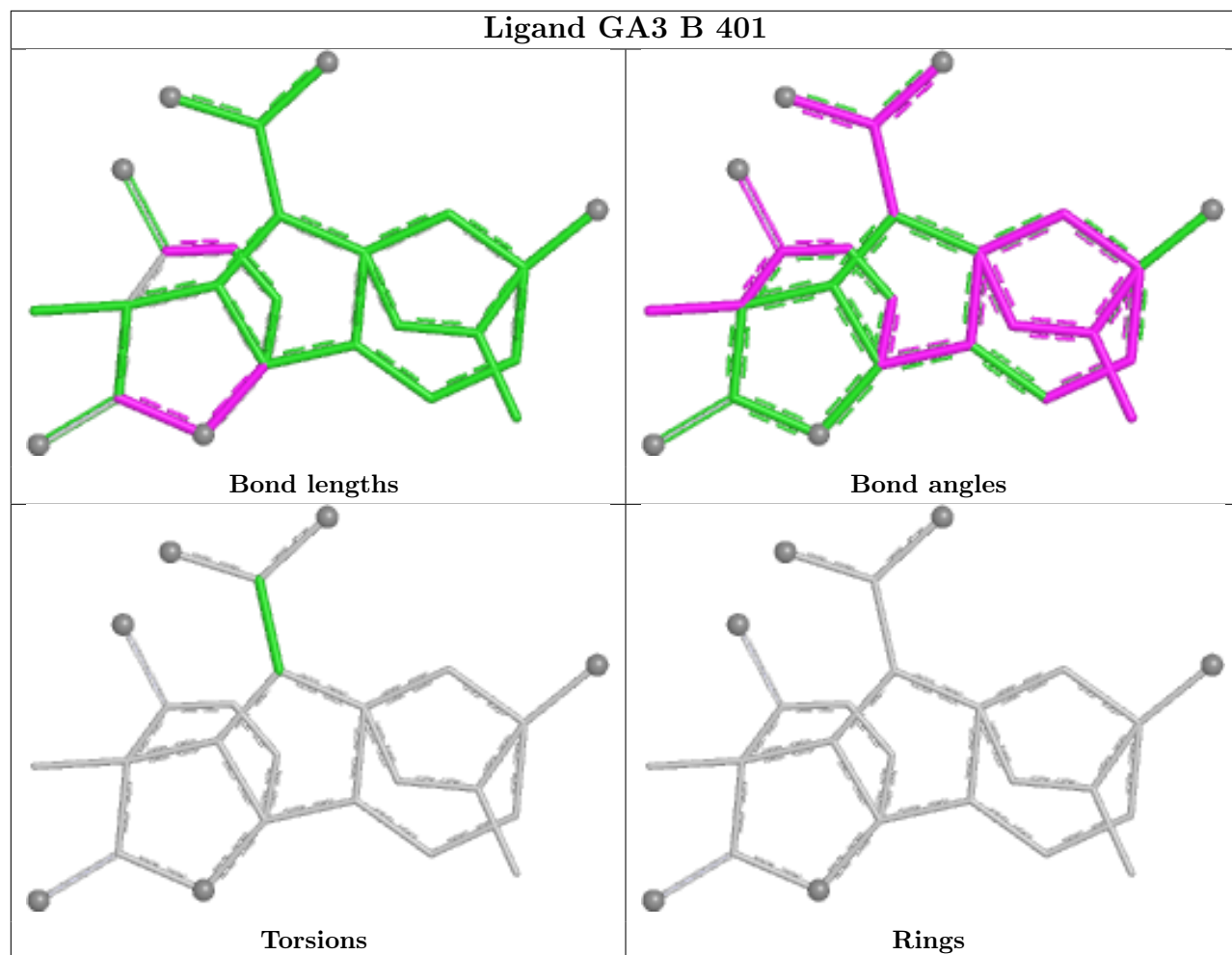
Ligand GA3 F 401

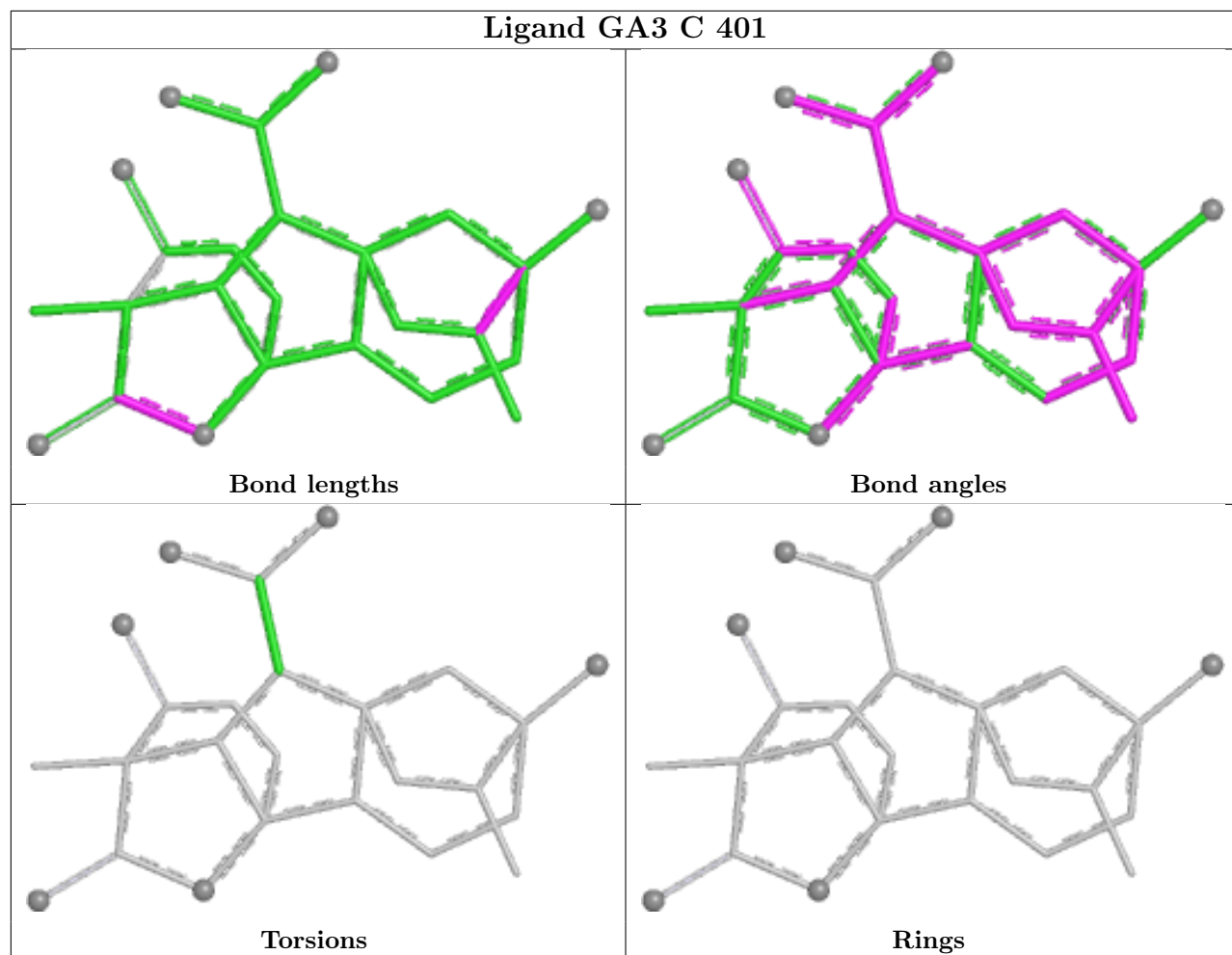


Ligand GA3 D 401



Ligand GA3 B 401





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	321/365 (87%)	-0.07	8 (2%) 58 62	11, 24, 42, 54	4 (1%)
1	B	316/365 (86%)	0.26	19 (6%) 27 29	12, 28, 49, 66	5 (1%)
1	C	301/365 (82%)	0.39	16 (5%) 32 34	14, 31, 48, 57	3 (0%)
1	D	315/365 (86%)	0.34	24 (7%) 20 21	15, 28, 48, 56	3 (0%)
1	E	313/365 (85%)	1.17	67 (21%) 2 2	22, 39, 56, 68	2 (0%)
1	F	305/365 (83%)	0.37	19 (6%) 26 28	16, 31, 50, 58	2 (0%)
All	All	1871/2190 (85%)	0.41	153 (8%) 17 18	11, 30, 51, 68	19 (1%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	PHE	5.5
1	E	181	PHE	5.3
1	E	188	ALA	4.9
1	D	280	LEU	4.9
1	F	74	VAL	4.4
1	C	282	GLY	4.3
1	E	110	ALA	4.3
1	D	274	GLY	4.3
1	D	313	GLY	4.3
1	B	104	LEU	4.0
1	A	15	VAL	4.0
1	E	106	ASP	4.0
1	A	105	THR	3.9
1	E	277	GLY	3.7
1	B	190	ALA	3.7
1	F	15	VAL	3.7
1	A	103	PHE	3.6
1	E	170	TRP	3.5
1	C	190	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	73	SER	3.5
1	D	74	VAL	3.5
1	D	73	SER	3.5
1	D	109	ALA	3.5
1	E	212	ALA	3.5
1	D	282	GLY	3.4
1	C	113	PHE	3.4
1	E	107	ALA	3.3
1	E	275	PRO	3.3
1	C	283	LEU	3.3
1	A	186	GLY	3.2
1	D	15	VAL	3.2
1	E	189	GLN	3.2
1	E	112	PRO	3.1
1	E	273	PHE	3.1
1	E	229	GLY	3.1
1	E	70	ILE	3.1
1	D	281	GLY	3.0
1	F	353	TYR	3.0
1	E	284	PRO	3.0
1	E	313	GLY	3.0
1	D	275	PRO	3.0
1	E	215	GLY	2.9
1	F	352	LEU	2.9
1	D	273	PHE	2.9
1	B	177	MET	2.9
1	A	353	TYR	2.9
1	F	215	GLY	2.9
1	E	209	VAL	2.8
1	E	272	PRO	2.8
1	D	72	GLN	2.8
1	B	181	PHE	2.8
1	C	181	PHE	2.8
1	D	310	ARG	2.8
1	E	283	LEU	2.8
1	C	180	PRO	2.8
1	E	15	VAL	2.8
1	E	216	VAL	2.8
1	E	203	ILE	2.8
1	E	74	VAL	2.8
1	E	184	SER	2.7
1	C	175	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	211	ALA	2.7
1	C	219	CYS	2.7
1	A	104	LEU	2.7
1	E	240	LEU	2.7
1	E	111	GLU	2.7
1	E	162	TYR	2.6
1	E	285	PHE	2.6
1	C	73	SER	2.6
1	B	109	ALA	2.6
1	E	308	ALA	2.6
1	B	180	PRO	2.6
1	E	268	PRO	2.6
1	E	303	LEU	2.6
1	E	108	PRO	2.6
1	F	72	GLN	2.6
1	B	277	GLY	2.6
1	E	315	HIS	2.5
1	C	277	GLY	2.5
1	B	107	ALA	2.5
1	F	349	ASN	2.5
1	F	190	ALA	2.5
1	D	162	TYR	2.5
1	E	230	GLY	2.5
1	F	274	GLY	2.5
1	E	72	GLN	2.5
1	C	170	TRP	2.5
1	E	264	ASP	2.5
1	F	216	VAL	2.5
1	E	180	PRO	2.5
1	E	113	PHE	2.4
1	F	66	PHE	2.4
1	E	260	PRO	2.4
1	E	309	LEU	2.4
1	E	263	ALA	2.4
1	E	349	ASN	2.4
1	B	60	LEU	2.4
1	B	215	GLY	2.4
1	E	280	LEU	2.3
1	D	84	ALA	2.3
1	E	109	ALA	2.3
1	F	57	ALA	2.3
1	E	75	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	274	GLY	2.3
1	E	281	GLY	2.3
1	E	279	ARG	2.3
1	B	14	THR	2.3
1	A	315	HIS	2.3
1	A	84	ALA	2.3
1	B	84	ALA	2.3
1	C	351	ASN	2.3
1	E	228	PHE	2.3
1	D	309	LEU	2.3
1	E	208	ALA	2.2
1	E	316	VAL	2.2
1	D	230	GLY	2.2
1	E	233	ARG	2.2
1	C	144	LEU	2.2
1	C	281	GLY	2.2
1	D	75	GLY	2.2
1	B	110	ALA	2.2
1	D	212	ALA	2.2
1	D	66	PHE	2.1
1	B	72	GLN	2.1
1	B	15	VAL	2.1
1	B	178	SER	2.1
1	B	75	GLY	2.1
1	E	299	CYS	2.1
1	E	177[A]	MET	2.1
1	E	190	ALA	2.1
1	F	181	PHE	2.1
1	E	258	TYR	2.1
1	F	70	ILE	2.1
1	D	279	ARG	2.1
1	E	169	GLY	2.1
1	D	315	HIS	2.1
1	E	76	LEU	2.1
1	F	60	LEU	2.1
1	F	275	PRO	2.1
1	C	193	PHE	2.1
1	F	273	PHE	2.1
1	E	262	ASP	2.1
1	E	301	ARG	2.1
1	F	278	ARG	2.1
1	E	234	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	268	PRO	2.0
1	E	191	ARG	2.0
1	E	257	ALA	2.0
1	E	276	ASN	2.0
1	B	74	VAL	2.0
1	C	74	VAL	2.0
1	E	207	VAL	2.0
1	E	218	VAL	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
3	NO3	A	601	4/4	0.77	0.20	45,45,46,46	0
5	PO4	B	701	5/5	0.78	0.18	89,89,89,90	0
3	NO3	D	601	4/4	0.80	0.14	61,61,61,61	0
3	NO3	A	602	4/4	0.81	0.15	42,43,44,45	0
2	MPD	D	501	8/8	0.83	0.13	34,38,38,40	0
3	NO3	B	601	4/4	0.84	0.15	49,50,50,51	0
3	NO3	F	602	4/4	0.87	0.21	51,51,51,53	0
3	NO3	B	604	4/4	0.87	0.21	50,51,51,51	0
5	PO4	E	701	5/5	0.87	0.17	97,98,98,98	0
3	NO3	A	603	4/4	0.88	0.12	61,61,62,62	0
3	NO3	F	603	4/4	0.88	0.10	62,62,62,62	0
3	NO3	B	602	4/4	0.88	0.16	45,46,46,46	0
2	MPD	B	501	8/8	0.88	0.11	33,36,36,37	0
3	NO3	C	602	4/4	0.89	0.17	42,43,43,43	0
3	NO3	D	603	4/4	0.91	0.10	51,51,51,52	0

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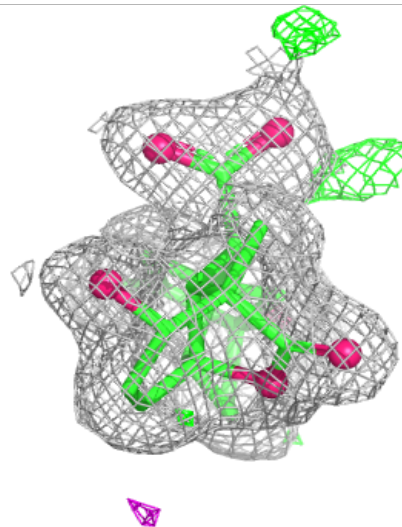
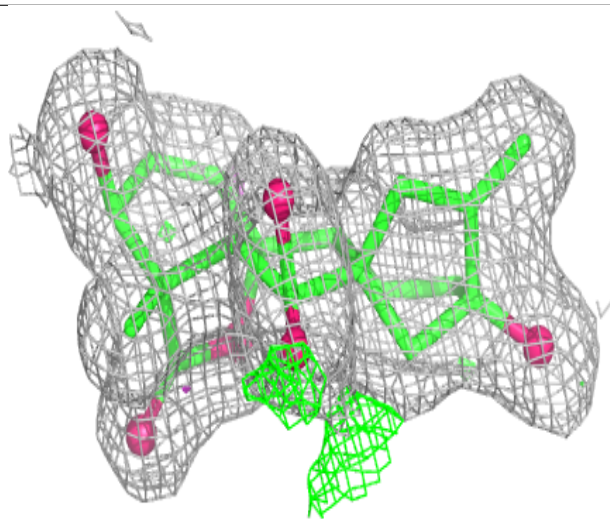
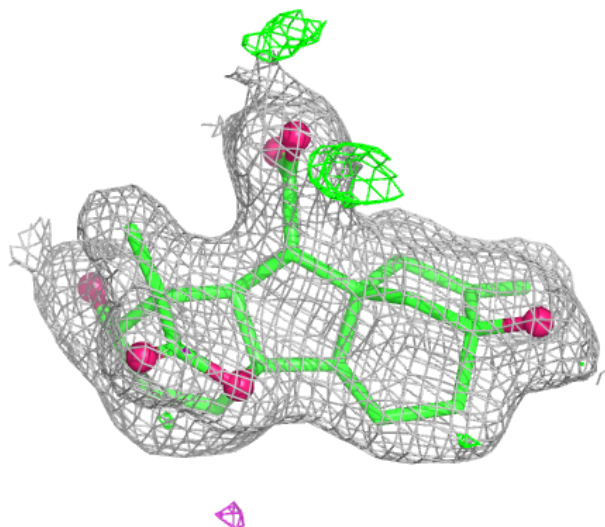
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MPD	A	501	8/8	0.91	0.13	28,31,37,37	0
3	NO3	C	604	4/4	0.91	0.14	44,45,45,46	0
2	MPD	F	501	8/8	0.92	0.10	32,34,35,35	0
2	MPD	C	501	8/8	0.93	0.09	31,33,35,35	0
4	GA3	E	401	25/25	0.93	0.07	24,28,30,32	0
2	MPD	E	501	8/8	0.94	0.10	38,41,42,43	0
4	GA3	F	401	25/25	0.96	0.06	20,23,26,27	0
4	GA3	C	401	25/25	0.97	0.05	16,19,22,23	0
4	GA3	D	401	25/25	0.97	0.05	19,21,23,26	0
4	GA3	B	401	25/25	0.97	0.05	15,17,21,21	0
4	GA3	A	401	25/25	0.98	0.04	15,17,20,20	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.

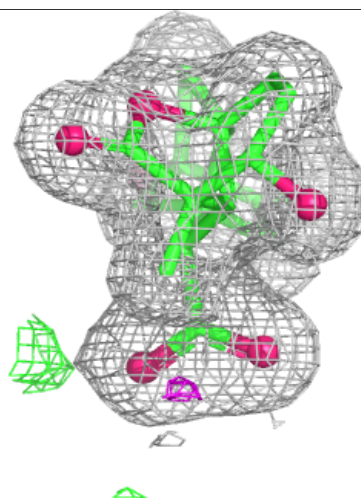
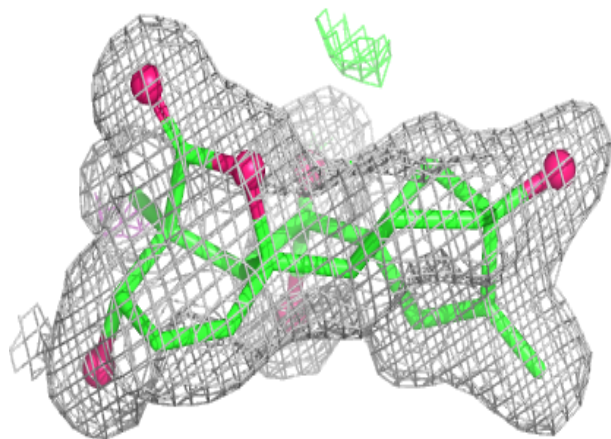
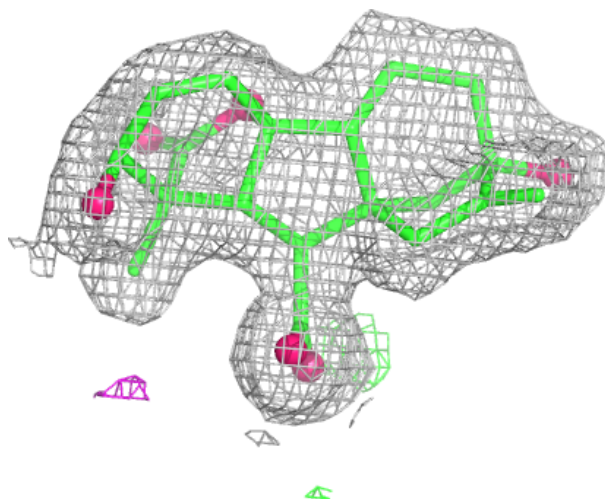
Electron density around GA3 E 401:

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



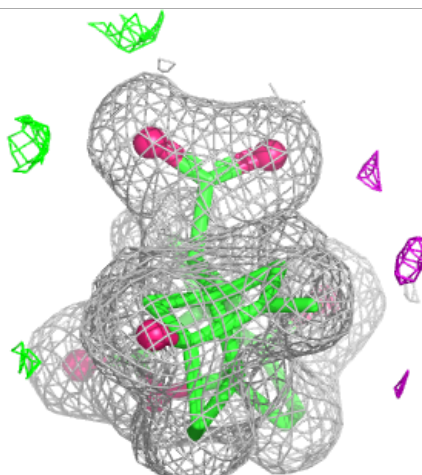
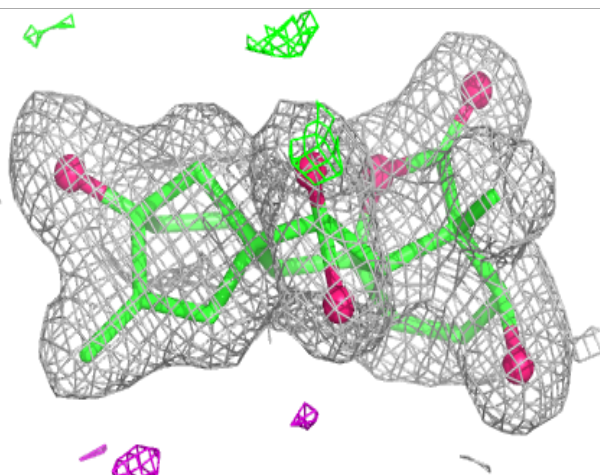
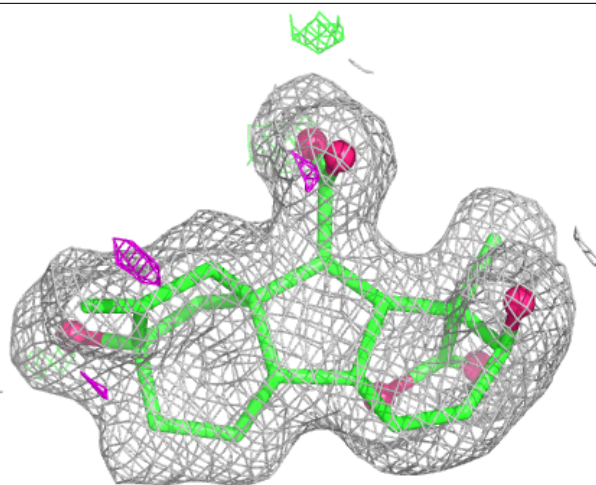
Electron density around GA3 F 401:

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



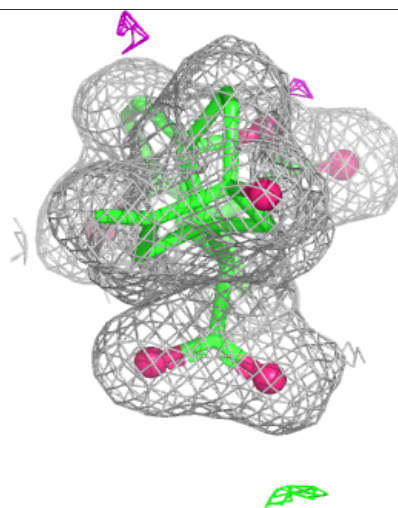
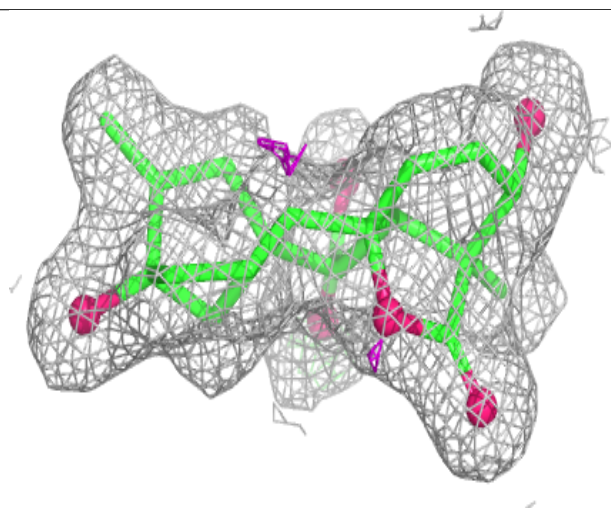
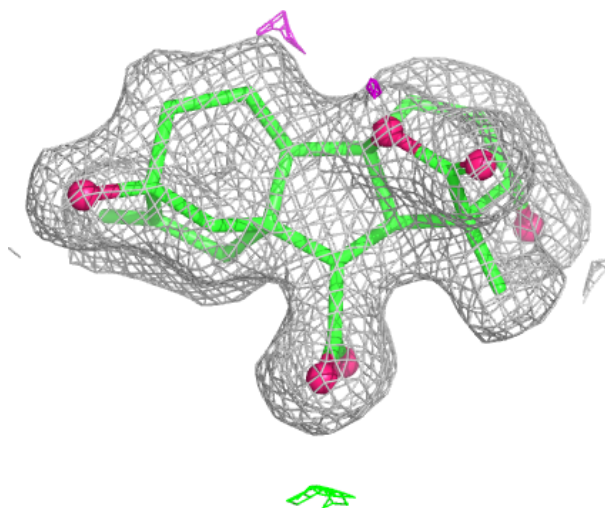
Electron density around GA3 C 401:

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



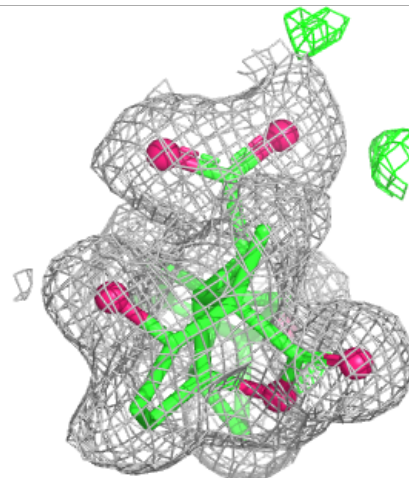
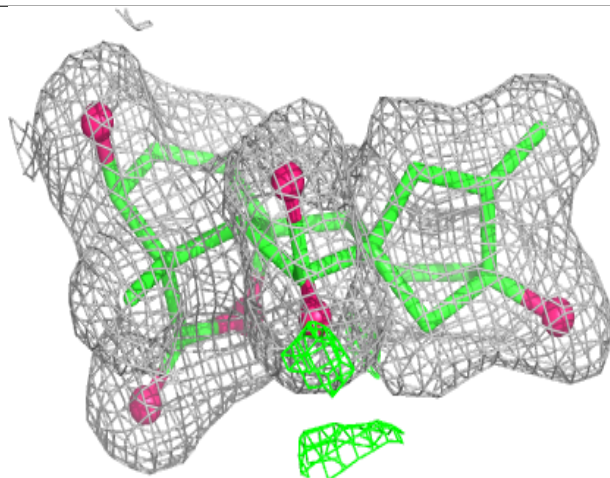
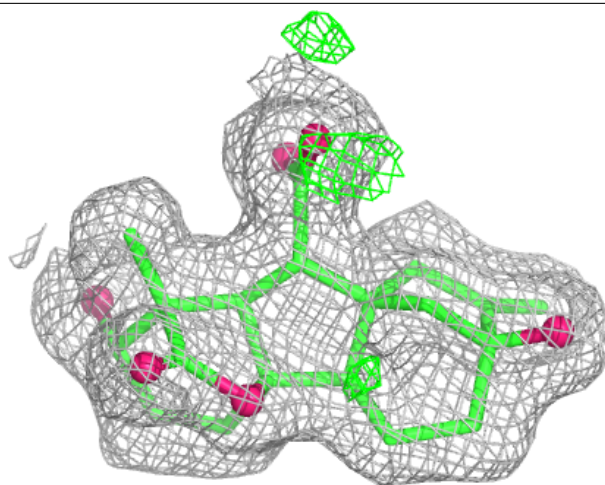
Electron density around GA3 D 401:

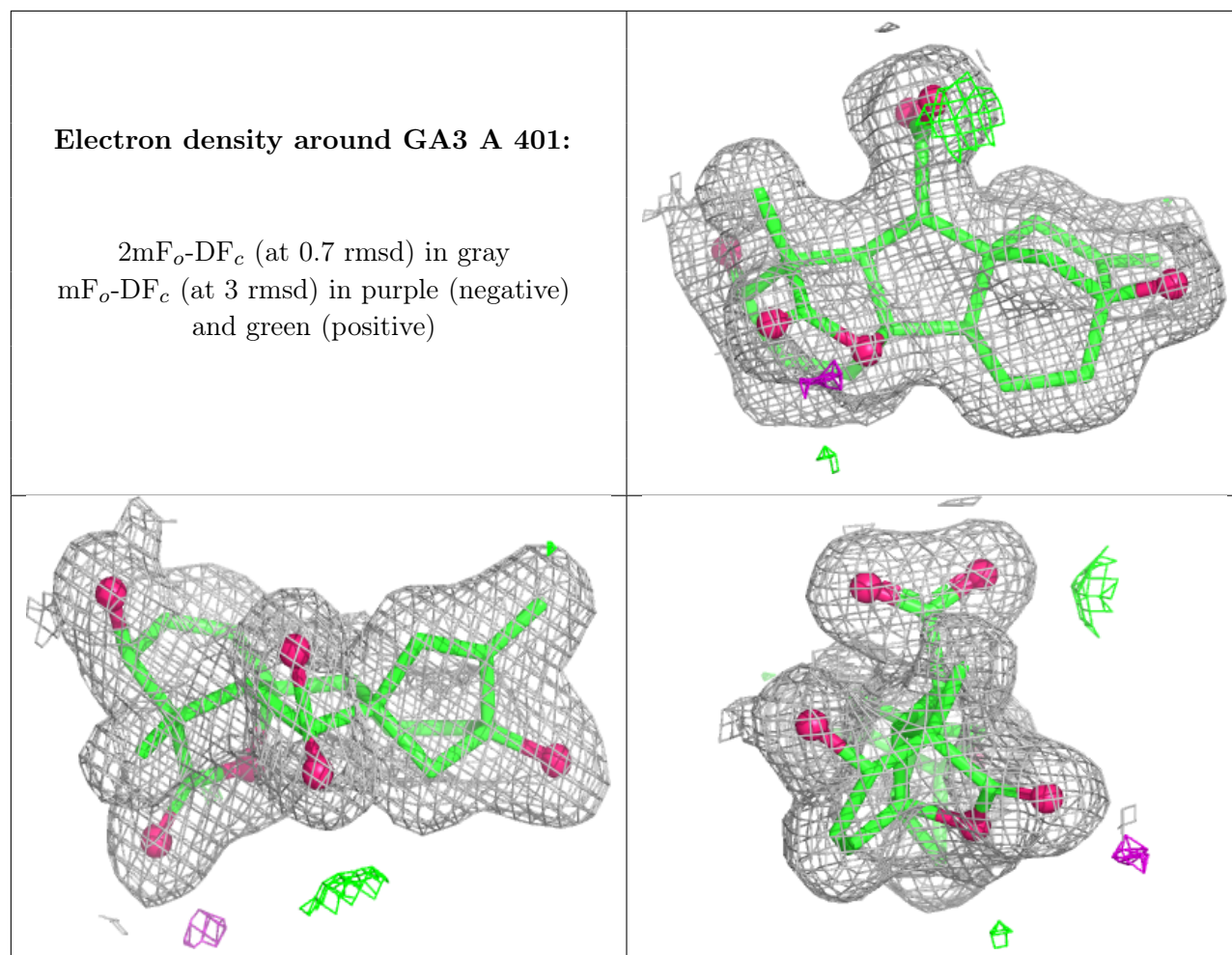
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GA3 B 401:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.