



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 03:14 PM EDT

PDB ID : 6KU3
Title : Crystal structure of gibberellin 2-oxidase3 (GA2ox3) in rice
Authors : Takehara, S.; Mikami, B.; Sakuraba, S.; Matsuoka, M.; Ueguchi-Tanaka, M.
Deposited on : 2019-08-30
Resolution : 2.15 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 : 2.37.1
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) : 2.37.1

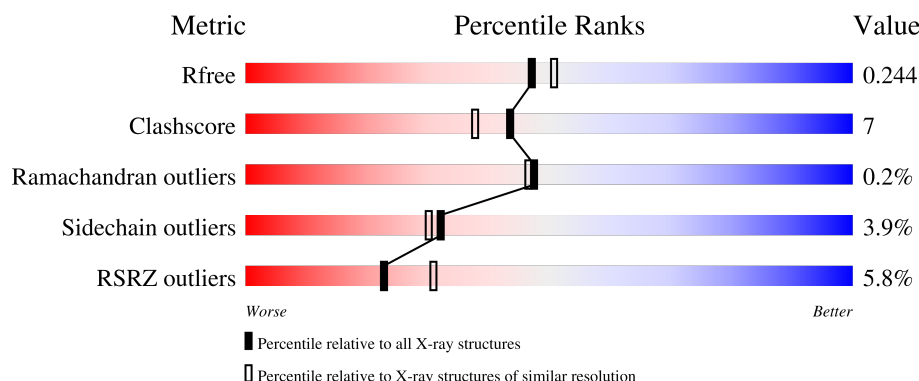
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


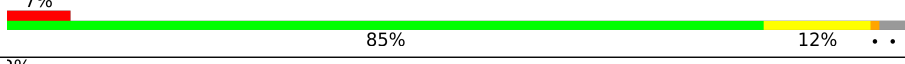


The reported resolution of this entry is 2.15 Å.

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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	327	
1	B	327	
1	C	327	
1	D	327	

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
3	AKG	D	402	-	X	X	-
4	GOL	B	405	-	-	-	X

2 Entry composition [i](#)

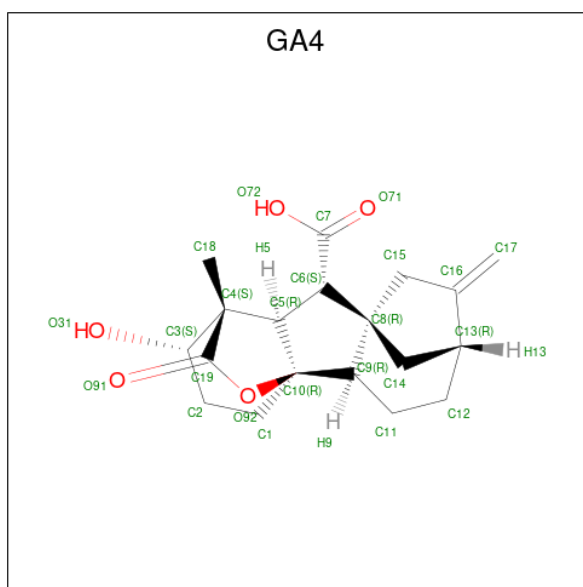
There are 6 unique types of molecules in this entry. The entry contains 10343 atoms, of which 20 are hydrogens and 0 are deuteriums.

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 2-beta-dioxygenase 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	317	Total	C	H	N	O	S	0	0	0
			2424	1530	3	425	457	9			
1	B	318	Total	C	N	O	S		0	0	0
			2431	1536	427	459	9				
1	C	317	Total	C	H	N	O	S	0	0	0
			2440	1531	17	426	457	9			
1	D	310	Total	C	N	O	S		0	0	0
			2372	1502	417	444	9				

- Molecule 2 is GIBBERELLIN A4 (three-letter code: GA4) (formula: C₁₉H₂₄O₅) (labeled as "Ligand of Interest" by depositor).



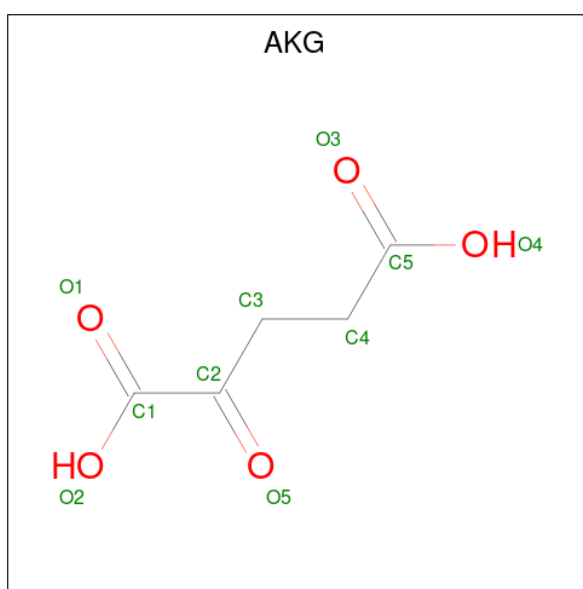
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			24	19	5		
2	A	1	Total	C	O	0	0
			24	19	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			24	19	5		
2	C	1	Total	C	O	0	0
			24	19	5		
2	C	1	Total	C	O	0	0
			24	19	5		
2	D	1	Total	C	O	0	0
			24	19	5		

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

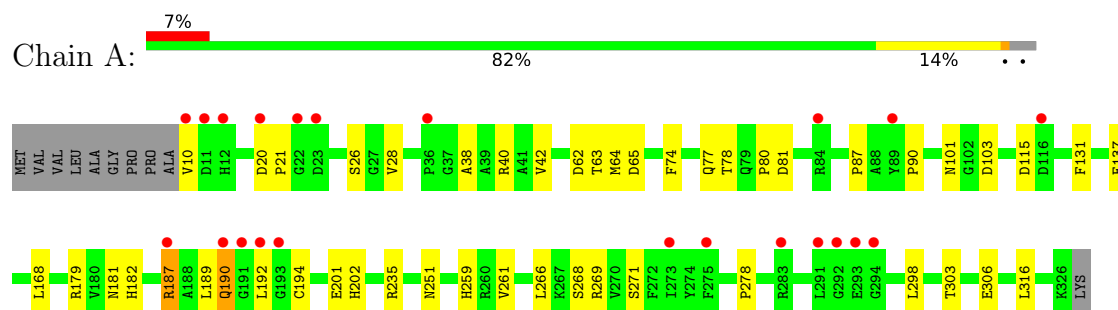
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	85	Total	O	0	0
			85	85		
6	B	126	Total	O	0	0
			126	126		
6	C	102	Total	O	0	0
			102	102		
6	D	89	Total	O	0	0
			89	89		

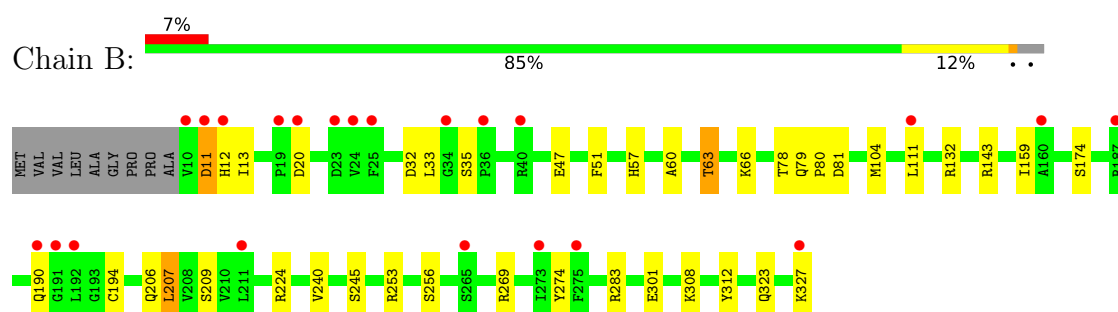
3 Residue-property plots [i](#)

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.

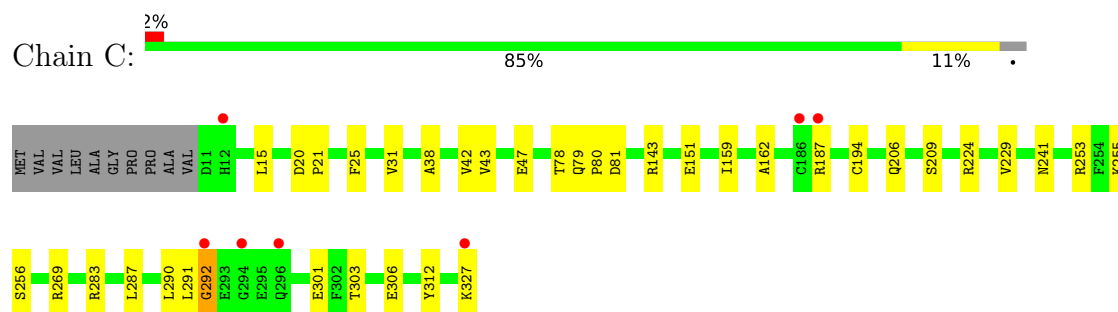
- Molecule 1: Gibberellin 2-beta-dioxygenase 3



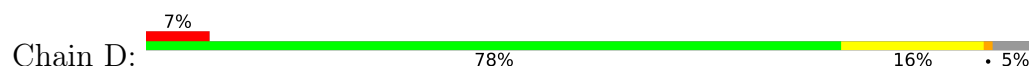
- Molecule 1: Gibberellin 2-beta-dioxygenase 3

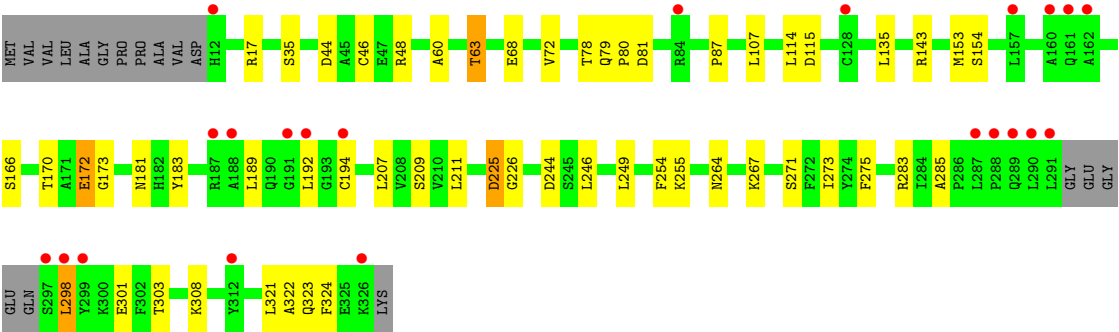


- Molecule 1: Gibberellin 2-beta-dioxygenase 3



- Molecule 1: Gibberellin 2-beta-dioxygenase 3





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.47Å 112.74Å 149.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.88 – 2.15 45.58 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.88-2.15) 99.8 (45.58-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.197 , 0.243 0.206 , 0.244	Depositor DCC
R_{free} test set	4591 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10343	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: SO4, GOL, GA4, AKG

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	0.59	0/2475	0.67	0/3355
1	B	0.60	0/2485	0.71	0/3368
1	C	0.58	0/2477	0.68	0/3356
1	D	0.59	0/2425	0.67	0/3287
All	All	0.59	0/9862	0.68	0/13366

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 [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	2421	3	2374	38	0
1	B	2431	0	2387	26	0
1	C	2423	17	2379	31	0
1	D	2372	0	2335	44	0
2	A	48	0	46	3	0
2	B	24	0	23	0	0
2	C	48	0	46	4	0
2	D	24	0	23	0	0
3	A	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	4	0	0
3	C	10	0	4	1	0
3	D	10	0	4	7	0
4	A	24	0	32	2	0
4	B	18	0	24	4	0
4	C	6	0	8	0	0
4	D	12	0	16	1	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	85	0	0	3	0
6	B	126	0	0	7	0
6	C	102	0	0	2	0
6	D	89	0	0	2	0
All	All	10323	20	9709	130	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 7.

All (130) 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:187:ARG:NH2	1:A:190:GLN:HG3	1.63	1.11
1:C:43:VAL:O	1:C:47:GLU:HG3	1.80	0.81
1:A:187:ARG:NH2	1:A:190:GLN:CG	2.46	0.78
1:C:194:CYS:HG	1:D:194:CYS:HG	1.09	0.76
4:B:405:GOL:H31	6:B:512:HOH:O	1.85	0.75
1:C:283:ARG:NH2	1:C:301:GLU:OE2	2.21	0.73
1:D:183:TYR:OH	3:D:402:AKG:H41	1.88	0.73
1:C:194:CYS:HG	1:D:194:CYS:CB	2.03	0.71
1:A:187:ARG:NH2	1:A:266:LEU:CD1	2.54	0.71
1:D:78:THR:HG23	1:D:81:ASP:H	1.56	0.71
1:A:187:ARG:HH21	1:A:190:GLN:HG3	1.54	0.70
2:A:401:GA4:O31	1:D:308:LYS:HE2	1.91	0.69
1:A:187:ARG:NH2	1:A:266:LEU:HD13	2.07	0.68
1:A:103:ASP:HB3	4:A:404:GOL:H12	1.76	0.68
1:C:303:THR:HG23	1:C:306:GLU:H	1.60	0.65
1:C:194:CYS:SG	1:D:194:CYS:CB	2.86	0.64
1:A:28:VAL:HG12	6:A:509:HOH:O	1.98	0.64
1:A:194:CYS:CB	1:B:194:CYS:SG	2.88	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASP:OD1	1:A:235:ARG:NH2	2.33	0.61
1:B:11:ASP:O	1:B:104:MET:HE1	2.01	0.60
4:B:404:GOL:H12	6:B:620:HOH:O	2.02	0.60
1:D:211:LEU:HD11	3:D:402:AKG:O4	2.02	0.59
1:A:194:CYS:SG	1:B:194:CYS:CB	2.90	0.59
1:C:194:CYS:SG	1:D:194:CYS:HB3	2.44	0.58
1:A:251:ASN:OD1	1:A:298:LEU:HD22	2.04	0.57
1:B:33:LEU:HB2	6:B:509:HOH:O	2.06	0.56
1:D:244:ASP:HB3	1:D:321:LEU:HD13	1.88	0.56
1:B:57:HIS:HA	6:B:509:HOH:O	2.04	0.56
1:C:78:THR:HG22	1:C:81:ASP:OD2	2.05	0.56
1:A:187:ARG:NH2	1:A:266:LEU:HD12	2.21	0.55
1:C:303:THR:HG22	1:C:306:GLU:CD	2.28	0.55
1:A:38:ALA:O	1:A:42:VAL:HG23	2.06	0.54
1:B:47:GLU:OE1	1:B:253:ARG:NE	2.36	0.54
2:A:401:GA4:O31	1:D:308:LYS:CE	2.56	0.54
1:B:327:LYS:HA	1:B:327:LYS:HE2	1.89	0.54
1:C:194:CYS:CB	1:D:194:CYS:HG	2.19	0.54
1:D:153:MET:HE3	1:D:246:LEU:HD21	1.90	0.54
1:D:273:ILE:HD11	3:D:402:AKG:H42	1.89	0.54
1:B:78:THR:HG23	1:B:81:ASP:H	1.72	0.54
1:A:90:PRO:HB3	2:A:401:GA4:O91	2.08	0.53
1:B:224:ARG:HE	4:B:404:GOL:C1	2.22	0.53
1:D:60:ALA:HB3	1:D:63:THR:HG22	1.91	0.53
1:D:143:ARG:NH2	1:D:170:THR:HA	2.23	0.53
1:A:179:ARG:HD3	1:A:181:ASN:HD21	1.75	0.52
1:C:290:LEU:N	1:C:290:LEU:HD12	2.24	0.51
1:A:78:THR:OG1	1:A:80:PRO:HD2	2.10	0.51
1:C:31:VAL:HG21	1:C:42:VAL:HG22	1.92	0.51
1:C:159:ILE:HD11	1:C:290:LEU:HD11	1.93	0.51
1:A:187:ARG:HH21	1:A:190:GLN:CG	2.18	0.51
1:A:261:VAL:HG23	6:A:553:HOH:O	2.11	0.51
1:B:60:ALA:HB3	1:B:63:THR:HG23	1.93	0.51
4:B:405:GOL:O1	2:C:402:GA4:H11	2.11	0.51
1:D:183:TYR:CE1	3:D:402:AKG:O3	2.64	0.50
1:A:101:ASN:OD1	1:D:87:PRO:HD2	2.11	0.50
1:D:46:CYS:HB3	1:D:254:PHE:CG	2.47	0.49
1:B:12:HIS:CG	1:B:13:ILE:H	2.31	0.49
1:B:66:LYS:HD2	6:B:547:HOH:O	2.13	0.49
1:D:181:ASN:HD22	3:D:402:AKG:H42	1.76	0.49
1:D:267:LYS:HE3	6:D:553:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ASP:O	1:B:104:MET:CE	2.59	0.49
1:D:68:GLU:O	1:D:72:VAL:HG23	2.12	0.49
1:D:283:ARG:NH2	1:D:301:GLU:OE1	2.46	0.49
1:C:78:THR:HG23	1:C:81:ASP:H	1.77	0.49
1:B:32:ASP:O	1:B:35:SER:HB3	2.12	0.49
1:C:287:LEU:HB2	1:C:290:LEU:HD13	1.94	0.48
1:D:225:ASP:N	1:D:225:ASP:OD1	2.46	0.48
1:C:209:SER:HB3	1:C:241:ASN:HB2	1.95	0.48
1:D:172:GLU:HG3	1:D:173:GLY:N	2.29	0.48
1:B:308:LYS:HE2	2:C:402:GA4:O31	2.14	0.48
1:C:78:THR:HG22	1:C:81:ASP:CG	2.33	0.48
1:C:291:LEU:O	1:C:292:GLY:O	2.31	0.48
1:A:64:MET:HE1	1:A:235:ARG:O	2.15	0.47
1:B:190:GLN:OE1	1:B:190:GLN:HA	2.14	0.47
1:D:207:LEU:HD22	1:D:249:LEU:HD12	1.95	0.47
1:D:153:MET:CE	1:D:246:LEU:HD21	2.44	0.47
1:D:298:LEU:CD1	1:D:298:LEU:N	2.78	0.47
1:A:189:LEU:HD23	1:A:192:LEU:HD12	1.95	0.46
1:D:271:SER:OG	3:D:402:AKG:O4	2.30	0.46
1:A:63:THR:HG23	1:A:137:GLU:HG2	1.96	0.46
1:A:298:LEU:HD22	1:A:298:LEU:H	1.78	0.46
1:C:194:CYS:CB	1:D:194:CYS:SG	3.03	0.46
1:D:298:LEU:N	1:D:298:LEU:HD12	2.30	0.46
1:A:78:THR:HG23	1:A:81:ASP:H	1.80	0.46
1:B:323:GLN:CB	6:B:584:HOH:O	2.63	0.46
1:B:207:LEU:HD13	1:B:245:SER:HB2	1.98	0.46
1:A:87:PRO:HD2	6:A:554:HOH:O	2.16	0.45
1:D:44:ASP:OD1	1:D:48:ARG:NH1	2.49	0.45
1:A:20:ASP:HB2	1:A:21:PRO:HD2	1.98	0.45
1:D:322:ALA:O	1:D:324:PHE:N	2.50	0.45
1:C:269:ARG:NH2	6:C:503:HOH:O	2.37	0.45
1:C:25:PHE:HB2	1:C:229:VAL:HB	1.98	0.44
1:A:316:LEU:HD23	4:A:404:GOL:H11	1.99	0.44
1:D:273:ILE:HD11	3:D:402:AKG:H31	1.99	0.44
1:A:303:THR:HG23	1:A:306:GLU:H	1.81	0.44
1:B:51:PHE:HA	1:B:240:VAL:O	2.17	0.44
1:D:79:GLN:HB3	1:D:80:PRO:HD3	1.99	0.44
1:A:251:ASN:OD1	1:A:298:LEU:CD2	2.65	0.44
1:D:249:LEU:HD23	1:D:285:ALA:O	2.17	0.44
1:A:187:ARG:CZ	1:A:266:LEU:HD12	2.47	0.44
1:C:151:GLU:HG2	1:C:162:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:LEU:O	6:D:501:HOH:O	2.21	0.43
1:B:33:LEU:CB	6:B:509:HOH:O	2.63	0.43
1:C:47:GLU:OE1	1:C:253:ARG:NE	2.48	0.43
1:A:194:CYS:HB3	1:B:194:CYS:SG	2.57	0.43
1:C:15:LEU:HD12	1:D:189:LEU:HD21	2.01	0.43
1:C:38:ALA:O	1:C:42:VAL:HG23	2.18	0.43
1:C:79:GLN:HB3	1:C:80:PRO:HD3	2.00	0.43
1:D:143:ARG:HH22	1:D:170:THR:HA	1.83	0.43
1:D:153:MET:HE3	1:D:254:PHE:HE2	1.84	0.43
1:C:303:THR:CG2	1:C:306:GLU:H	2.31	0.42
1:A:74:PHE:O	1:A:77:GLN:HB2	2.18	0.42
1:A:202:HIS:HB3	1:A:316:LEU:HG	2.01	0.42
1:D:225:ASP:HB2	1:D:226:GLY:CA	2.49	0.42
1:B:209:SER:HA	1:B:274:TYR:O	2.20	0.42
1:B:312:TYR:CD2	2:C:402:GA4:H3	2.54	0.42
1:D:264:ASN:ND2	4:D:404:GOL:H2	2.35	0.42
1:B:283:ARG:NH2	1:B:301:GLU:OE2	2.52	0.41
1:C:224:ARG:NH2	6:C:511:HOH:O	2.52	0.41
1:D:135:LEU:HD23	1:D:135:LEU:HA	1.92	0.41
1:A:168:LEU:O	1:A:278:PRO:HA	2.21	0.41
1:C:20:ASP:HB2	1:C:21:PRO:HD2	2.01	0.41
1:B:79:GLN:HB3	1:B:80:PRO:HD3	2.03	0.41
1:A:194:CYS:SG	1:B:194:CYS:HB3	2.59	0.41
1:A:201:GLU:HA	1:A:259:HIS:O	2.21	0.41
1:A:182:HIS:NE2	1:A:268:SER:OG	2.48	0.41
1:A:187:ARG:HH22	1:A:266:LEU:HD13	1.80	0.40
1:D:189:LEU:HA	1:D:192:LEU:HD12	2.03	0.40
1:D:209:SER:HB3	1:D:275:PHE:CD1	2.56	0.40
1:C:312:TYR:CD1	2:C:402:GA4:H171	2.56	0.40
1:C:269:ARG:NH1	3:C:403:AKG:O4	2.54	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	315/327 (96%)	301 (96%)	14 (4%)	0	100	100
1	B	316/327 (97%)	305 (96%)	10 (3%)	1 (0%)	41	37
1	C	315/327 (96%)	303 (96%)	11 (4%)	1 (0%)	41	37
1	D	306/327 (94%)	293 (96%)	13 (4%)	0	100	100
All	All	1252/1308 (96%)	1202 (96%)	48 (4%)	2 (0%)	47	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	292	GLY
1	B	174	SER

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	257/264 (97%)	247 (96%)	10 (4%)	32	30
1	B	258/264 (98%)	247 (96%)	11 (4%)	29	27
1	C	257/264 (97%)	251 (98%)	6 (2%)	50	53
1	D	252/264 (96%)	239 (95%)	13 (5%)	23	19
All	All	1024/1056 (97%)	984 (96%)	40 (4%)	32	30

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	26	SER
1	A	40	ARG
1	A	62	ASP
1	A	115	ASP
1	A	131	PHE

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Mol	Chain	Res	Type
1	A	187	ARG
1	A	190	GLN
1	A	269	ARG
1	A	271	SER
1	B	11	ASP
1	B	20	ASP
1	B	63	THR
1	B	111	LEU
1	B	132	ARG
1	B	143	ARG
1	B	159	ILE
1	B	206	GLN
1	B	207	LEU
1	B	256	SER
1	B	269	ARG
1	C	143	ARG
1	C	187	ARG
1	C	206	GLN
1	C	255	LYS
1	C	256	SER
1	C	327	LYS
1	D	17	ARG
1	D	35	SER
1	D	63	THR
1	D	107	LEU
1	D	115	ASP
1	D	154	SER
1	D	166	SER
1	D	172	GLU
1	D	225	ASP
1	D	255	LYS
1	D	298	LEU
1	D	303	THR
1	D	323	GLN

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	$\# Z > 2$
5	SO4	C	405	-	4,4,4	0.26	0	6,6,6	0.34	0
4	GOL	B	403	-	5,5,5	0.34	0	5,5,5	1.35	0
4	GOL	A	406	-	5,5,5	0.83	0	5,5,5	0.81	0
4	GOL	B	405	-	5,5,5	0.26	0	5,5,5	0.28	0
5	SO4	A	408	-	4,4,4	0.47	0	6,6,6	0.63	0
4	GOL	C	404	-	5,5,5	0.60	0	5,5,5	0.56	0
3	AKG	D	402	-	9,9,9	2.83	3 (33%)	11,11,11	4.18	7 (63%)
2	GA4	C	401	-	28,28,28	2.61	11 (39%)	42,49,49	1.81	8 (19%)
4	GOL	A	407	-	5,5,5	1.16	0	5,5,5	1.17	1 (20%)
2	GA4	A	402	-	28,28,28	2.56	11 (39%)	42,49,49	1.85	11 (26%)
4	GOL	A	404	-	5,5,5	1.52	1 (20%)	5,5,5	0.90	0
4	GOL	D	404	-	5,5,5	0.39	0	5,5,5	1.31	0
4	GOL	D	403	-	5,5,5	0.25	0	5,5,5	0.28	0
3	AKG	C	403	-	9,9,9	1.62	2 (22%)	11,11,11	2.45	8 (72%)
2	GA4	B	401	-	28,28,28	1.32	2 (7%)	42,49,49	2.04	11 (26%)
4	GOL	A	405	-	5,5,5	0.74	0	5,5,5	1.15	0
5	SO4	B	406	-	4,4,4	0.17	0	6,6,6	0.28	0
3	AKG	A	403	-	9,9,9	1.99	3 (33%)	11,11,11	1.93	5 (45%)
2	GA4	A	401	-	28,28,28	1.33	2 (7%)	42,49,49	2.05	10 (23%)
5	SO4	A	409	-	4,4,4	0.67	0	6,6,6	1.33	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	D	405	-	4,4,4	0.22	0	6,6,6	0.29	0
5	SO4	A	410	-	4,4,4	0.33	0	6,6,6	0.05	0
2	GA4	D	401	-	28,28,28	2.58	12 (42%)	42,49,49	1.75	9 (21%)
2	GA4	C	402	-	28,28,28	1.33	2 (7%)	42,49,49	2.05	10 (23%)
3	AKG	B	402	-	9,9,9	2.24	5 (55%)	11,11,11	1.72	2 (18%)
4	GOL	B	404	-	5,5,5	1.20	0	5,5,5	0.99	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
4	GOL	B	403	-	-	0/4/4/4	-
4	GOL	A	406	-	-	4/4/4/4	-
4	GOL	B	405	-	-	2/4/4/4	-
4	GOL	C	404	-	-	2/4/4/4	-
3	AKG	D	402	-	-	6/9/9/9	-
2	GA4	C	401	-	-	0/4/80/80	-
4	GOL	A	407	-	-	2/4/4/4	-
2	GA4	A	402	-	-	0/4/80/80	-
4	GOL	A	404	-	-	4/4/4/4	-
4	GOL	D	404	-	-	4/4/4/4	-
4	GOL	D	403	-	-	2/4/4/4	-
3	AKG	C	403	-	-	1/9/9/9	-
2	GA4	B	401	-	-	0/4/80/80	-
4	GOL	A	405	-	-	3/4/4/4	-
3	AKG	A	403	-	-	1/9/9/9	-
2	GA4	A	401	-	-	0/4/80/80	-
2	GA4	D	401	-	-	0/4/80/80	-
2	GA4	C	402	-	-	0/4/80/80	-
3	AKG	B	402	-	-	3/9/9/9	-
4	GOL	B	404	-	-	0/4/4/4	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	GA4	O92-C10	-8.52	1.35	1.47
2	D	401	GA4	O92-C10	-7.90	1.36	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	GA4	O92-C10	-7.88	1.36	1.47
3	D	402	AKG	C3-C2	5.37	1.57	1.51
3	D	402	AKG	C2-C1	4.91	1.60	1.53
2	D	401	GA4	C13-C16	-4.89	1.44	1.51
2	C	401	GA4	C13-C16	-4.51	1.45	1.51
3	A	403	AKG	O1-C1	4.22	1.33	1.22
2	C	402	GA4	O92-C19	4.21	1.44	1.36
2	A	401	GA4	O92-C19	4.19	1.44	1.36
2	B	401	GA4	O92-C19	4.18	1.44	1.36
3	B	402	AKG	O1-C1	4.06	1.33	1.22
2	D	401	GA4	C4-C19	-3.92	1.46	1.52
2	A	402	GA4	C13-C16	-3.73	1.46	1.51
2	A	402	GA4	C14-C8	-3.72	1.48	1.54
2	C	401	GA4	C4-C19	-3.64	1.46	1.52
2	C	401	GA4	O31-C3	-3.56	1.37	1.43
2	C	401	GA4	O72-C7	-3.51	1.19	1.30
2	D	401	GA4	O31-C3	-3.40	1.38	1.43
2	A	402	GA4	C15-C8	-3.40	1.49	1.55
2	A	402	GA4	O72-C7	-3.28	1.19	1.30
2	A	402	GA4	C4-C19	-3.18	1.47	1.52
2	A	401	GA4	O92-C10	-3.08	1.43	1.47
2	B	401	GA4	O92-C10	-3.06	1.43	1.47
2	C	402	GA4	O92-C10	-3.05	1.43	1.47
2	D	401	GA4	O72-C7	-3.02	1.20	1.30
3	C	403	AKG	C2-C1	2.97	1.57	1.53
2	D	401	GA4	C14-C8	-2.96	1.49	1.54
3	B	402	AKG	C4-C5	2.90	1.57	1.50
2	C	401	GA4	C15-C8	-2.89	1.50	1.55
2	C	401	GA4	C14-C8	-2.88	1.49	1.54
3	D	402	AKG	O4-C5	-2.87	1.21	1.30
2	A	402	GA4	O31-C3	-2.86	1.38	1.43
2	D	401	GA4	O91-C19	-2.82	1.14	1.20
2	D	401	GA4	C15-C8	-2.78	1.50	1.55
2	A	402	GA4	C10-C5	-2.74	1.48	1.54
4	A	404	GOL	C1-C2	2.71	1.62	1.51
2	C	401	GA4	C4-C5	-2.63	1.48	1.54
2	A	402	GA4	O91-C19	-2.51	1.15	1.20
2	D	401	GA4	C10-C9	-2.50	1.48	1.53
2	D	401	GA4	C10-C5	-2.47	1.49	1.54
2	A	402	GA4	C18-C4	-2.33	1.50	1.54
3	B	402	AKG	C3-C2	2.30	1.53	1.51
2	C	401	GA4	C18-C4	-2.30	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	GA4	C15-C16	-2.25	1.48	1.51
3	B	402	AKG	O4-C5	-2.23	1.23	1.30
3	A	403	AKG	O4-C5	-2.21	1.23	1.30
3	A	403	AKG	C4-C5	2.17	1.55	1.50
3	C	403	AKG	O1-C1	2.15	1.28	1.22
2	D	401	GA4	C18-C4	-2.12	1.50	1.54
2	A	402	GA4	C15-C16	-2.08	1.48	1.51
2	D	401	GA4	C4-C5	-2.08	1.49	1.54
3	B	402	AKG	C2-C1	2.02	1.56	1.53
2	C	401	GA4	O91-C19	-2.01	1.16	1.20

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	AKG	C3-C2-C1	8.49	131.72	115.97
2	C	402	GA4	C15-C16-C13	6.91	112.84	107.41
2	A	401	GA4	C15-C16-C13	6.88	112.81	107.41
2	B	401	GA4	C15-C16-C13	6.85	112.79	107.41
2	A	402	GA4	C15-C16-C13	6.84	112.78	107.41
2	C	401	GA4	C15-C16-C13	6.63	112.62	107.41
2	A	401	GA4	C14-C8-C15	5.96	105.61	100.17
2	B	401	GA4	C14-C8-C15	5.90	105.56	100.17
2	C	402	GA4	C14-C8-C15	5.86	105.53	100.17
3	D	402	AKG	O2-C1-C2	5.26	128.37	113.97
3	D	402	AKG	O5-C2-C3	-5.25	109.57	121.20
3	D	402	AKG	O4-C5-O3	-4.97	110.92	123.30
2	D	401	GA4	C15-C16-C13	4.70	111.10	107.41
2	D	401	GA4	O92-C10-C1	-4.45	104.55	107.32
3	D	402	AKG	O2-C1-O1	-4.23	113.93	123.61
2	A	401	GA4	O92-C10-C5	3.96	105.21	101.62
2	C	402	GA4	O92-C10-C5	3.93	105.18	101.62
2	B	401	GA4	O92-C10-C5	3.88	105.14	101.62
2	D	401	GA4	C5-C4-C19	-3.84	96.14	100.53
2	A	402	GA4	O92-C10-C9	3.73	113.07	108.68
3	B	402	AKG	O4-C5-O3	-3.65	114.21	123.30
2	C	401	GA4	C13-C16-C17	-3.56	122.53	126.12
3	D	402	AKG	O4-C5-C4	3.41	125.00	114.03
3	C	403	AKG	O1-C1-C2	-3.39	117.20	121.72
2	C	401	GA4	C14-C13-C16	-3.36	98.34	102.24
2	D	401	GA4	O92-C10-C9	3.36	112.64	108.68
2	C	401	GA4	O92-C10-C9	3.23	112.48	108.68
3	B	402	AKG	C3-C2-C1	3.07	121.67	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	AKG	O1-C1-C2	-3.07	117.63	121.72
3	C	403	AKG	O2-C1-C2	3.05	122.30	113.97
2	C	401	GA4	C1-C2-C3	3.01	116.05	111.51
3	C	403	AKG	O5-C2-C1	3.00	123.77	119.43
2	C	402	GA4	C1-C2-C3	2.97	116.00	111.51
2	A	401	GA4	C1-C2-C3	2.91	115.91	111.51
2	A	402	GA4	C5-C4-C19	-2.88	97.24	100.53
2	B	401	GA4	C1-C2-C3	2.87	115.85	111.51
2	C	401	GA4	O92-C10-C1	-2.81	105.57	107.32
3	A	403	AKG	C3-C2-C1	2.80	121.17	115.97
3	A	403	AKG	O4-C5-O3	-2.79	116.34	123.30
2	A	402	GA4	C14-C13-C16	-2.78	99.01	102.24
3	C	403	AKG	O4-C5-C4	2.74	122.82	114.03
2	C	402	GA4	O92-C10-C1	2.67	108.98	107.32
2	A	402	GA4	C8-C15-C16	-2.67	99.59	104.58
2	A	402	GA4	C2-C3-C4	-2.64	108.84	112.32
3	C	403	AKG	O5-C2-C3	-2.63	115.38	121.20
3	C	403	AKG	C3-C2-C1	2.63	120.85	115.97
2	A	401	GA4	O92-C10-C1	2.62	108.95	107.32
2	C	401	GA4	C5-C4-C19	-2.62	97.54	100.53
2	B	401	GA4	O92-C10-C1	2.61	108.94	107.32
2	C	402	GA4	C13-C16-C17	-2.56	123.54	126.12
2	A	401	GA4	C13-C16-C17	-2.54	123.56	126.12
2	B	401	GA4	C8-C15-C16	-2.51	99.90	104.58
2	C	402	GA4	C8-C15-C16	-2.51	99.90	104.58
3	A	403	AKG	O5-C2-C1	2.50	123.05	119.43
2	A	401	GA4	C8-C15-C16	-2.49	99.94	104.58
3	A	403	AKG	O5-C2-C3	-2.45	115.77	121.20
2	A	402	GA4	C1-C2-C3	2.44	115.20	111.51
2	B	401	GA4	C13-C16-C17	-2.44	123.67	126.12
2	A	402	GA4	C13-C16-C17	-2.44	123.67	126.12
2	A	401	GA4	O92-C19-O91	2.40	124.66	121.55
2	B	401	GA4	O92-C19-O91	2.39	124.65	121.55
3	A	403	AKG	C3-C4-C5	-2.39	108.47	113.60
2	D	401	GA4	C13-C16-C17	-2.36	123.74	126.12
3	C	403	AKG	O4-C5-O3	-2.35	117.45	123.30
2	C	402	GA4	O92-C19-O91	2.34	124.58	121.55
2	C	402	GA4	C6-C8-C9	2.26	108.91	104.24
2	A	401	GA4	C6-C8-C9	2.25	108.90	104.24
2	B	401	GA4	C6-C8-C9	2.23	108.85	104.24
2	D	401	GA4	O92-C10-C5	2.23	103.64	101.62
5	A	409	SO4	O3-S-O1	-2.20	97.81	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	GA4	C18-C4-C3	2.19	114.33	110.99
2	A	402	GA4	C10-C5-C6	-2.19	101.69	104.08
2	C	402	GA4	C18-C4-C3	2.18	114.32	110.99
2	D	401	GA4	C1-C2-C3	2.17	114.79	111.51
2	A	401	GA4	C18-C4-C3	2.17	114.30	110.99
2	C	401	GA4	O72-C7-O71	-2.15	119.20	124.09
2	D	401	GA4	C11-C9-C10	-2.13	112.09	118.31
5	A	409	SO4	O4-S-O1	2.13	120.42	109.31
2	D	401	GA4	O91-C19-C4	-2.09	124.44	128.64
3	C	403	AKG	C3-C4-C5	-2.08	109.14	113.60
4	A	407	GOL	C3-C2-C1	-2.06	103.70	111.70
2	A	402	GA4	O92-C10-C1	-2.03	106.05	107.32
2	A	402	GA4	C15-C16-C17	-2.02	123.54	126.31
2	B	401	GA4	C15-C16-C17	-2.02	123.54	126.31

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	AKG	C2-C3-C4-C5
3	D	402	AKG	O1-C1-C2-C3
3	D	402	AKG	O2-C1-C2-C3
4	A	404	GOL	O1-C1-C2-C3
4	A	407	GOL	C1-C2-C3-O3
4	B	405	GOL	C1-C2-C3-O3
4	D	403	GOL	O1-C1-C2-C3
4	D	404	GOL	O1-C1-C2-C3
4	D	404	GOL	C1-C2-C3-O3
4	A	404	GOL	O2-C2-C3-O3
4	C	404	GOL	O2-C2-C3-O3
4	A	404	GOL	C1-C2-C3-O3
4	A	405	GOL	C1-C2-C3-O3
4	A	406	GOL	O1-C1-C2-C3
4	A	406	GOL	C1-C2-C3-O3
4	C	404	GOL	C1-C2-C3-O3
4	A	404	GOL	O1-C1-C2-O2
4	A	406	GOL	O1-C1-C2-O2
4	A	407	GOL	O2-C2-C3-O3
4	B	405	GOL	O2-C2-C3-O3
4	D	404	GOL	O1-C1-C2-O2
4	D	404	GOL	O2-C2-C3-O3
4	D	403	GOL	O1-C1-C2-O2

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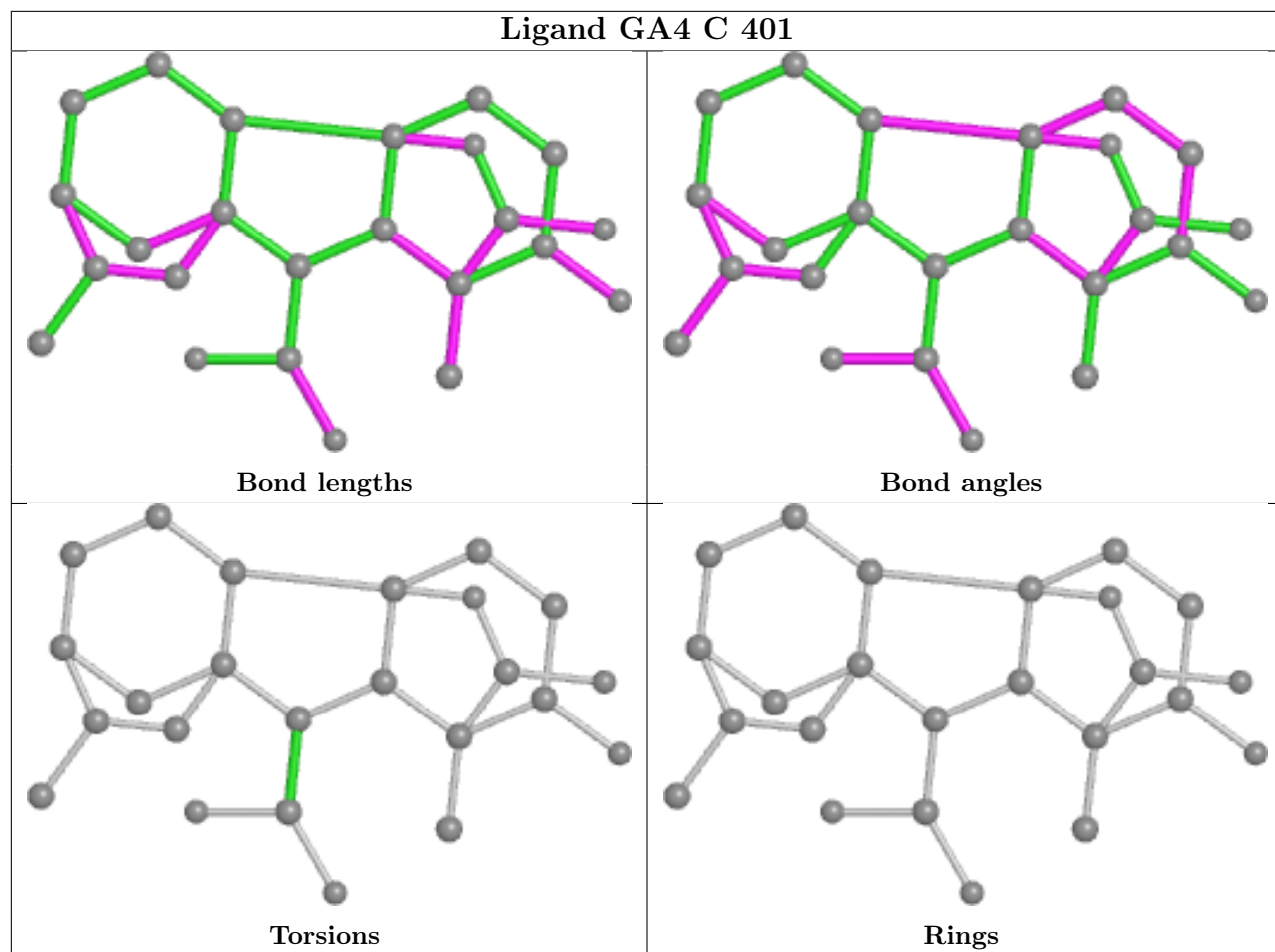
Mol	Chain	Res	Type	Atoms
3	D	402	AKG	O1-C1-C2-O5
4	A	405	GOL	O2-C2-C3-O3
3	D	402	AKG	C3-C4-C5-O3
3	B	402	AKG	C2-C3-C4-C5
3	C	403	AKG	C2-C3-C4-C5
3	D	402	AKG	C3-C4-C5-O4
4	A	405	GOL	O1-C1-C2-C3
4	A	406	GOL	O2-C2-C3-O3
3	D	402	AKG	O5-C2-C3-C4
3	B	402	AKG	C3-C4-C5-O3
3	B	402	AKG	C3-C4-C5-O4

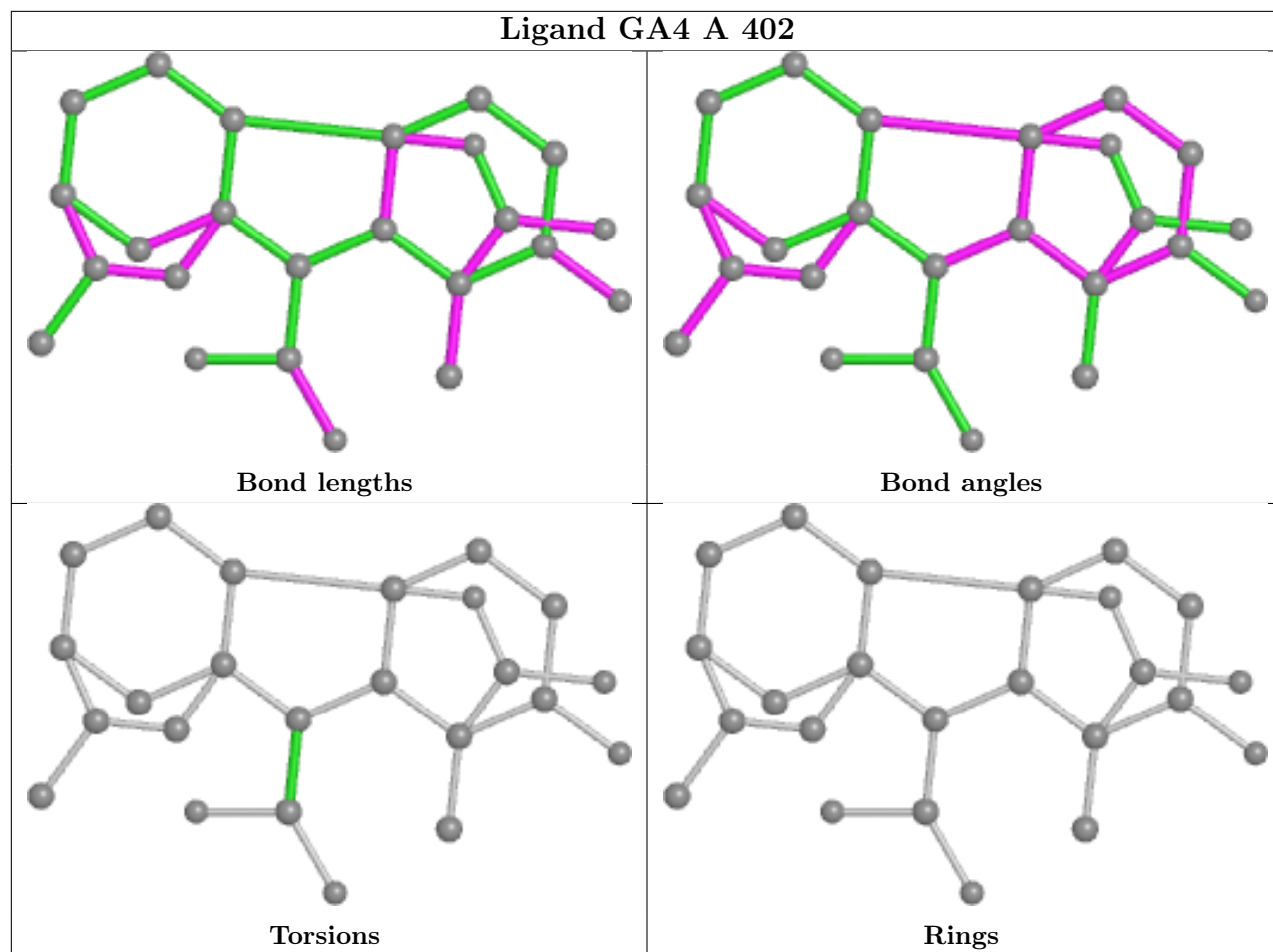
There are no ring outliers.

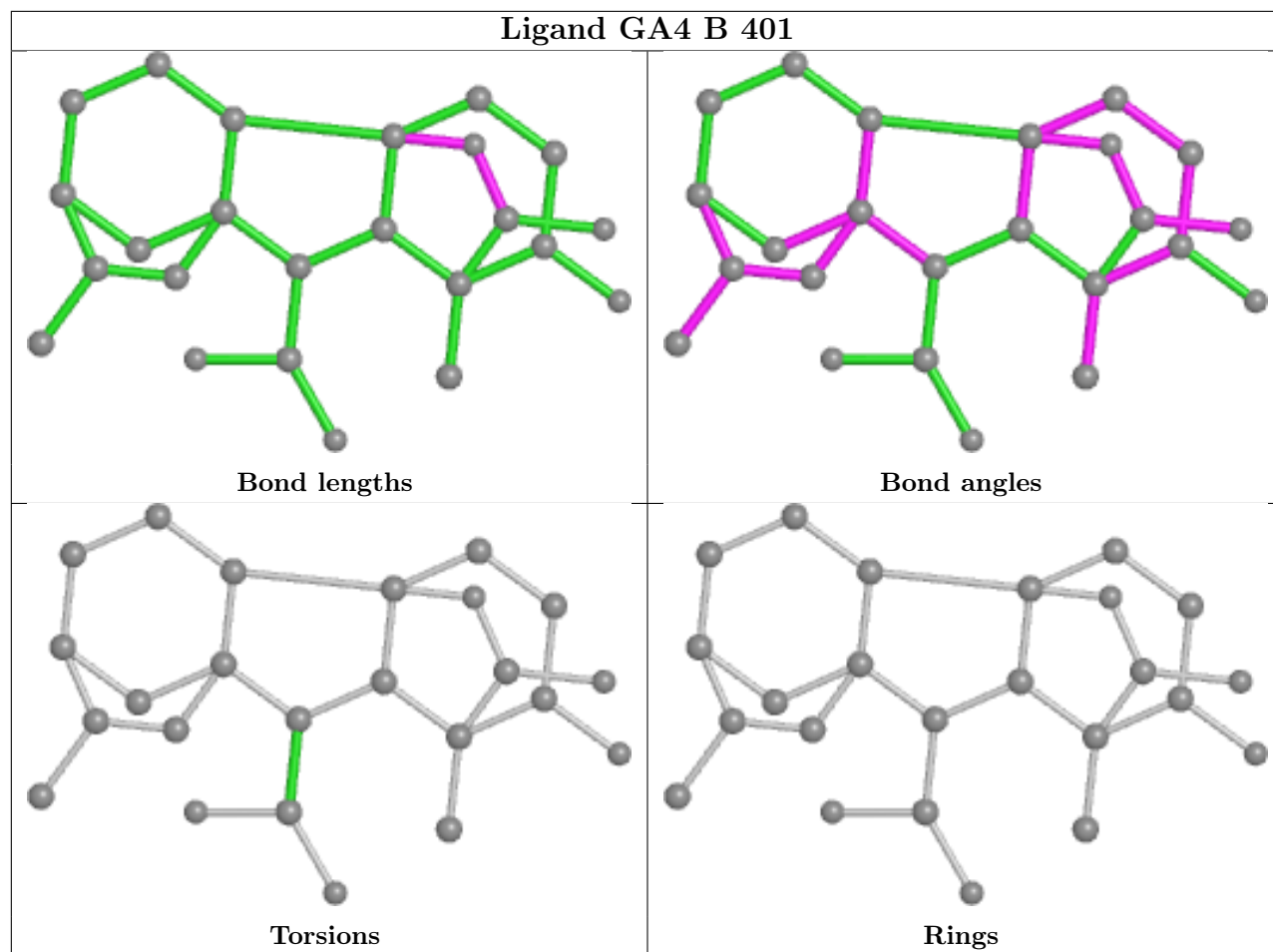
8 monomers are involved in 21 short contacts:

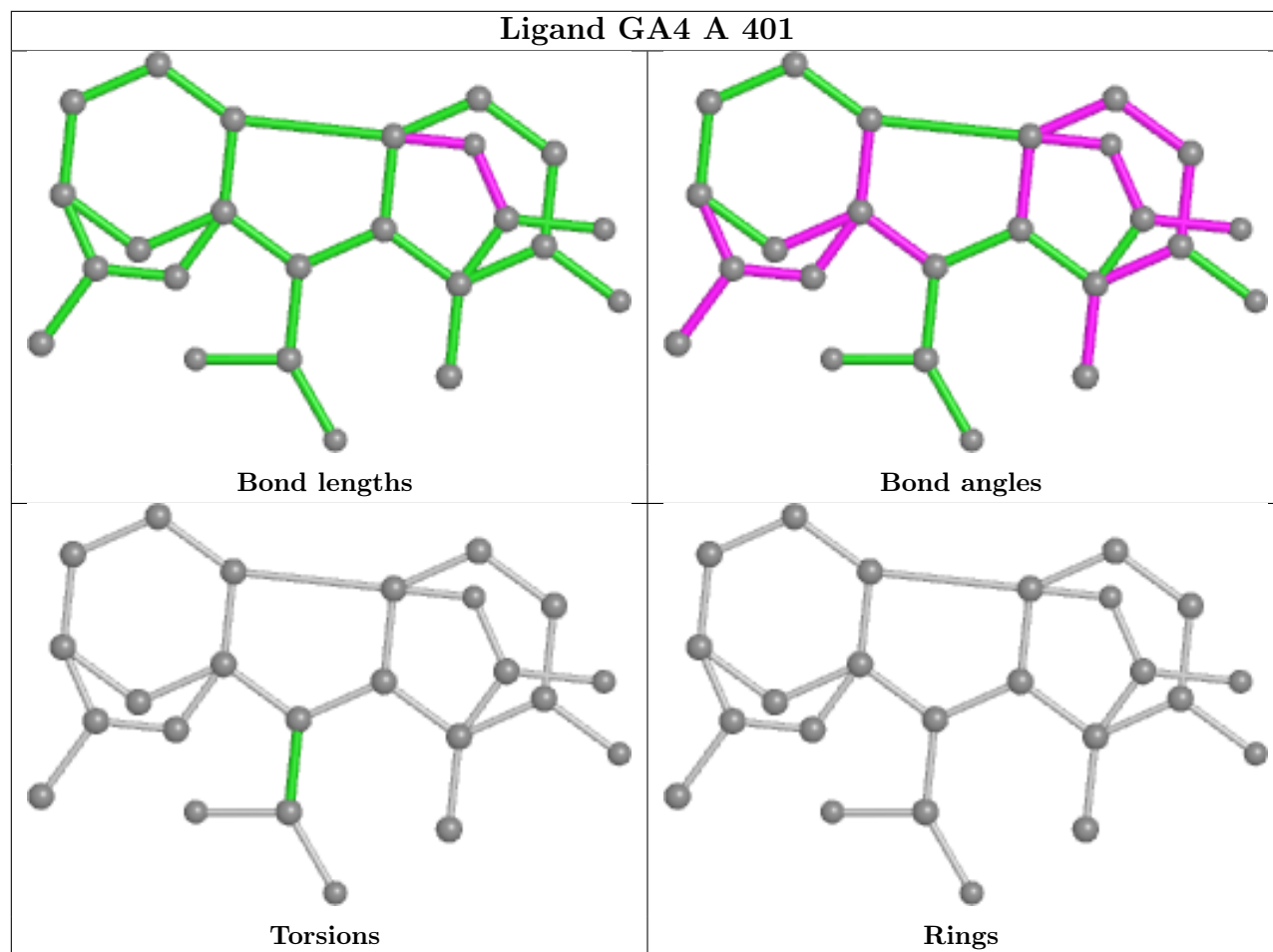
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	405	GOL	2	0
3	D	402	AKG	7	0
4	A	404	GOL	2	0
4	D	404	GOL	1	0
3	C	403	AKG	1	0
2	A	401	GA4	3	0
2	C	402	GA4	4	0
4	B	404	GOL	2	0

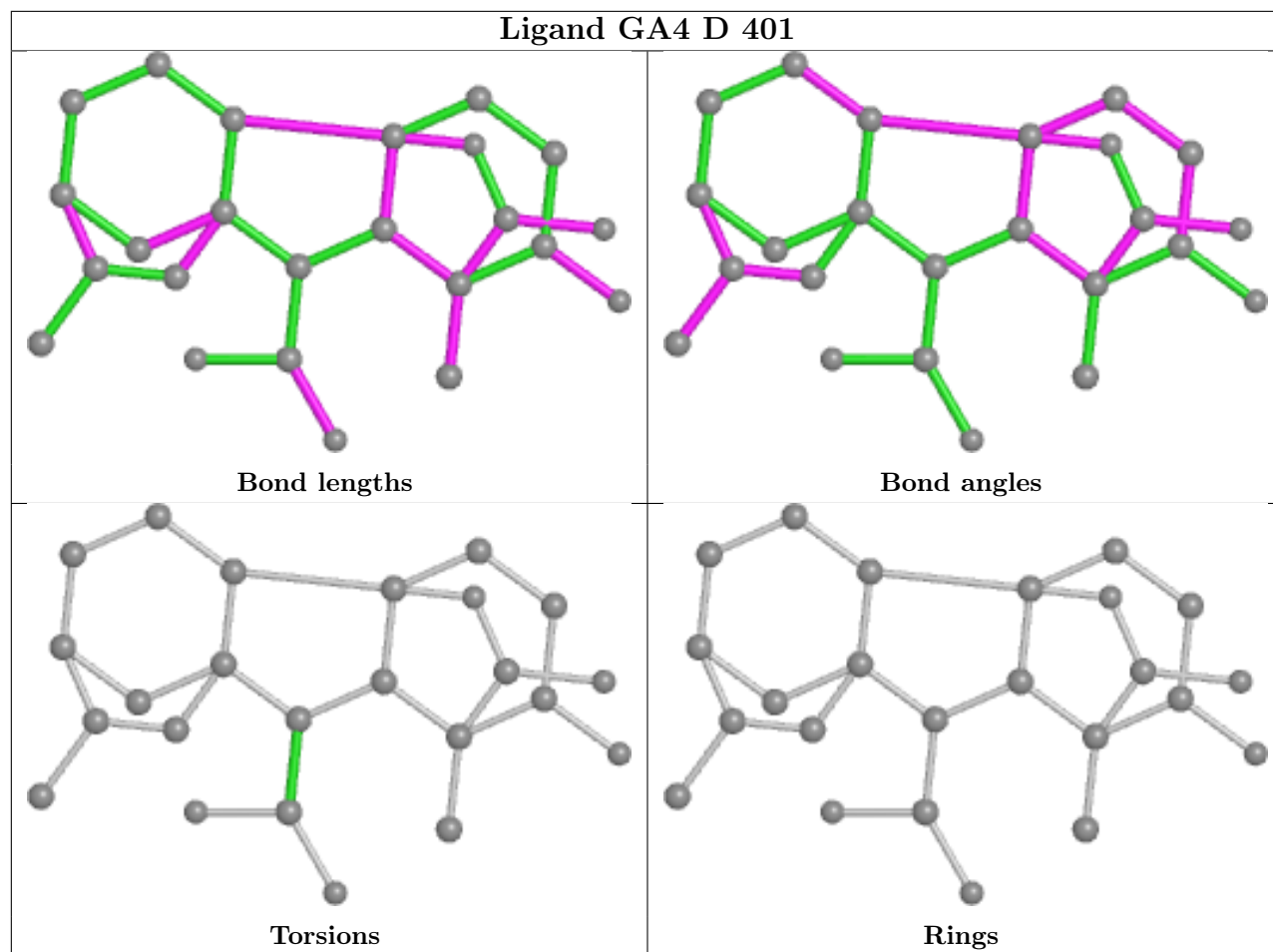
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

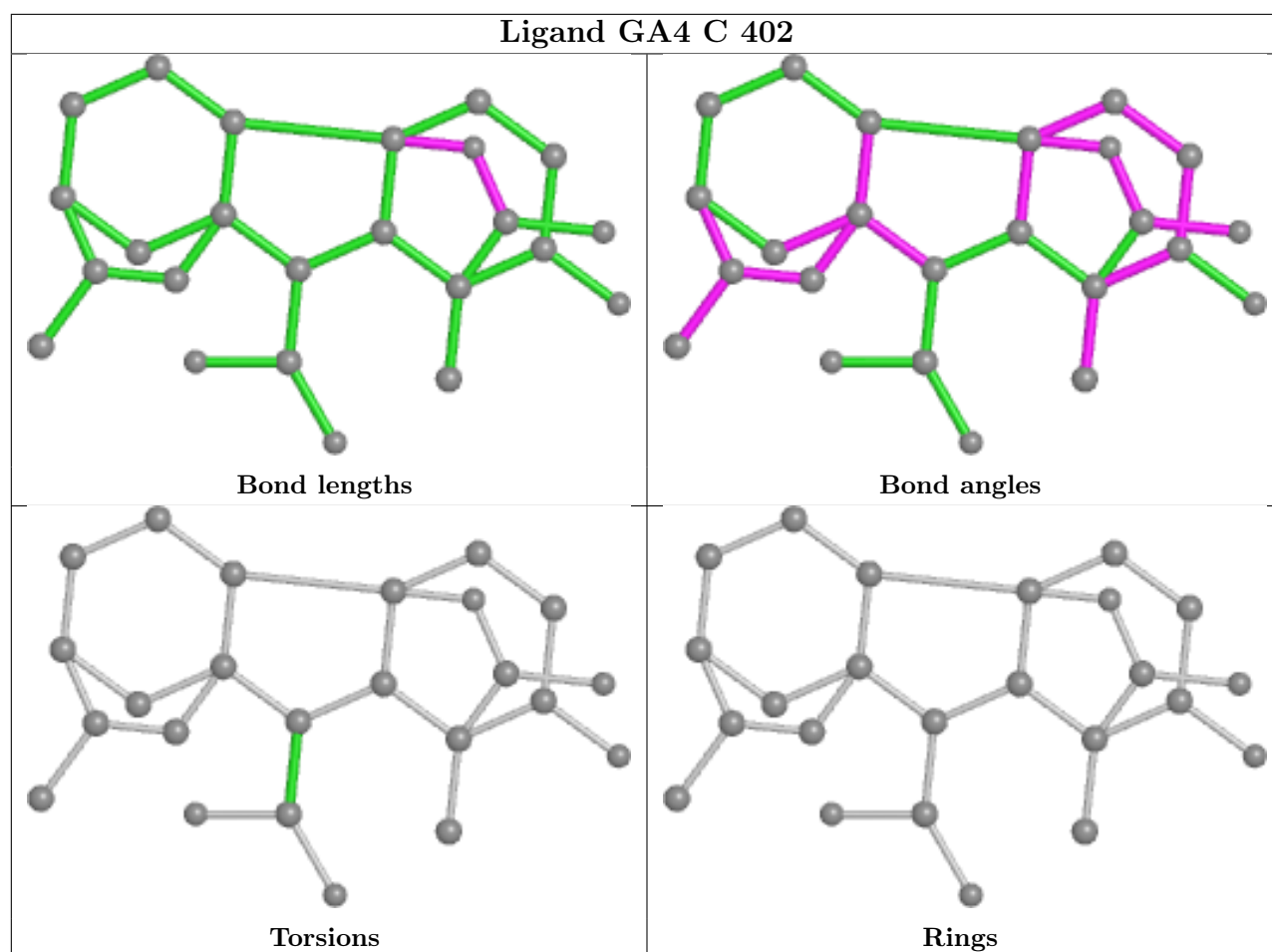












5.7 Other polymers [i](#)

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	317/327 (96%)	0.33	22 (6%) 16 23	26, 43, 73, 104	0
1	B	318/327 (97%)	0.35	22 (6%) 16 23	25, 40, 66, 96	0
1	C	317/327 (96%)	-0.04	7 (2%) 62 69	27, 40, 63, 87	0
1	D	310/327 (94%)	0.33	22 (7%) 16 22	27, 45, 67, 79	0
All	All	1262/1308 (96%)	0.24	73 (5%) 23 31	25, 42, 67, 104	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	VAL	8.2
1	B	12	HIS	6.4
1	D	290	LEU	5.2
1	A	294	GLY	5.1
1	A	292	GLY	5.0
1	B	187	ARG	4.9
1	B	11	ASP	4.8
1	A	187	ARG	4.8
1	B	191	GLY	4.7
1	A	293	GLU	4.7
1	C	327	LYS	4.6
1	C	294	GLY	4.3
1	A	283	ARG	3.8
1	A	11	ASP	3.7
1	A	23	ASP	3.7
1	D	288	PRO	3.7
1	B	34	GLY	3.6
1	D	160	ALA	3.5
1	D	12	HIS	3.5
1	D	291	LEU	3.5
1	C	187	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	192	LEU	3.3
1	C	12	HIS	3.1
1	D	188	ALA	3.1
1	B	211	LEU	3.1
1	D	191	GLY	3.0
1	D	289	GLN	3.0
1	A	291	LEU	3.0
1	D	298	LEU	2.9
1	D	187	ARG	2.8
1	B	10	VAL	2.8
1	D	194	CYS	2.8
1	B	20	ASP	2.7
1	B	23	ASP	2.7
1	D	162	ALA	2.7
1	D	287	LEU	2.7
1	C	292	GLY	2.7
1	D	299	TYR	2.7
1	D	192	LEU	2.6
1	A	193	GLY	2.6
1	B	275	PHE	2.6
1	B	111	LEU	2.6
1	A	190	GLN	2.6
1	B	25	PHE	2.6
1	A	12	HIS	2.5
1	D	84	ARG	2.5
1	A	116	ASP	2.5
1	D	161	GLN	2.5
1	A	191	GLY	2.5
1	D	297	SER	2.4
1	B	192	LEU	2.4
1	A	36	PRO	2.4
1	B	327	LYS	2.4
1	B	40	ARG	2.4
1	A	20	ASP	2.4
1	A	22	GLY	2.3
1	B	265	SER	2.3
1	D	312	TYR	2.3
1	B	273	ILE	2.2
1	A	84	ARG	2.2
1	B	160	ALA	2.2
1	D	128	CYS	2.1
1	B	36	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	326	LYS	2.1
1	B	24	VAL	2.1
1	B	190	GLN	2.1
1	D	157	LEU	2.1
1	A	275	PHE	2.1
1	C	296	GLN	2.1
1	A	89	TYR	2.1
1	A	273	ILE	2.0
1	B	19	PRO	2.0
1	C	186	CYS	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 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, 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
4	GOL	B	405	6/6	0.63	1.17	106,141,156,207	0
4	GOL	D	403	6/6	0.63	0.22	61,67,75,85	0
4	GOL	A	406	6/6	0.64	0.31	78,80,82,86	0
4	GOL	A	407	6/6	0.78	0.24	52,55,66,67	0
2	GA4	A	401	24/24	0.80	0.30	44,59,67,69	0
5	SO4	D	405	5/5	0.81	0.29	63,66,82,103	0
5	SO4	A	410	5/5	0.84	0.46	30,30,30,30	0
4	GOL	A	404	6/6	0.85	0.26	30,49,56,59	0
5	SO4	B	406	5/5	0.85	0.31	69,82,105,106	0
4	GOL	B	403	6/6	0.85	0.14	49,55,59,60	0
3	AKG	D	402	10/10	0.86	0.26	25,43,52,63	0
5	SO4	C	405	5/5	0.86	0.33	67,67,86,104	0
3	AKG	C	403	10/10	0.86	0.28	29,42,59,69	0

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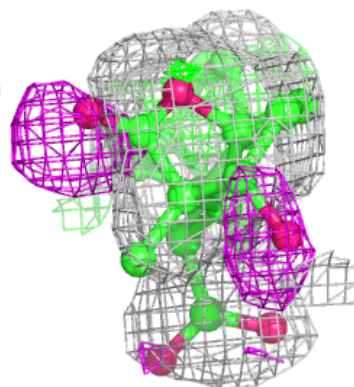
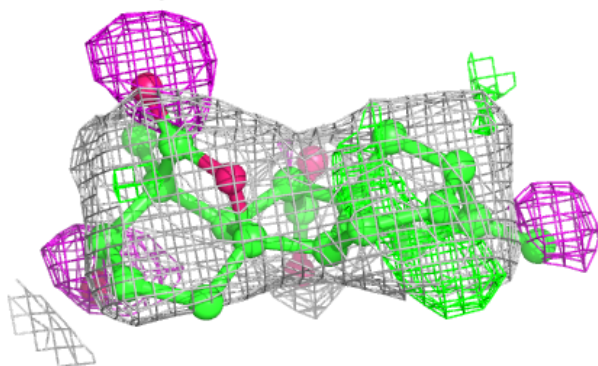
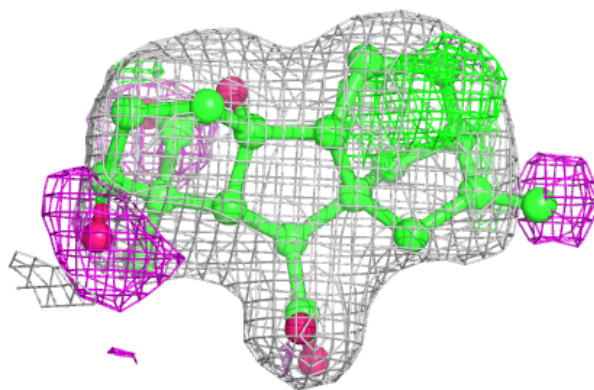
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	C	404	6/6	0.87	0.19	50,60,61,71	0
3	AKG	B	402	10/10	0.88	0.25	22,44,59,65	0
3	AKG	A	403	10/10	0.89	0.21	24,41,57,69	0
2	GA4	B	401	24/24	0.89	0.25	19,27,34,36	0
2	GA4	C	402	24/24	0.89	0.30	51,67,76,81	0
4	GOL	B	404	6/6	0.90	0.22	39,58,63,65	0
4	GOL	D	404	6/6	0.90	0.14	42,53,60,61	0
5	SO4	A	409	5/5	0.91	0.32	55,73,99,102	0
5	SO4	A	408	5/5	0.93	0.20	68,71,82,98	0
4	GOL	A	405	6/6	0.95	0.12	33,44,51,55	0
2	GA4	A	402	24/24	0.96	0.23	23,34,39,41	0
2	GA4	C	401	24/24	0.97	0.14	23,29,36,42	0
2	GA4	D	401	24/24	0.97	0.21	24,31,37,40	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.

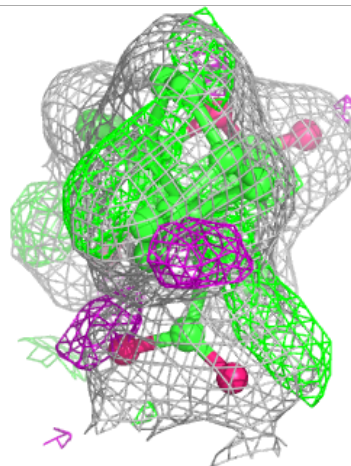
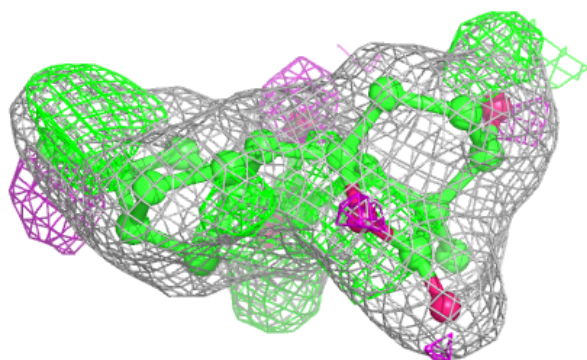
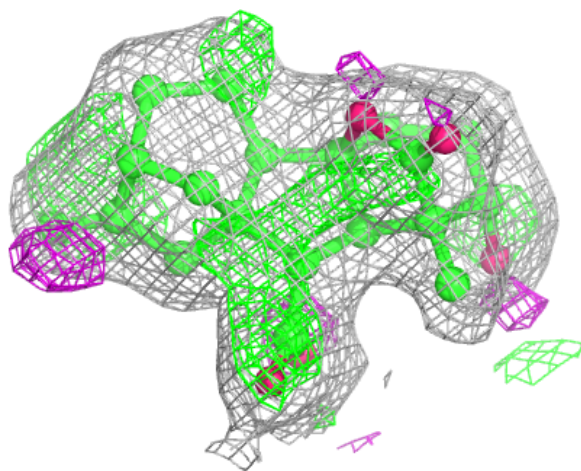
Electron density around GA4 A 401:

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



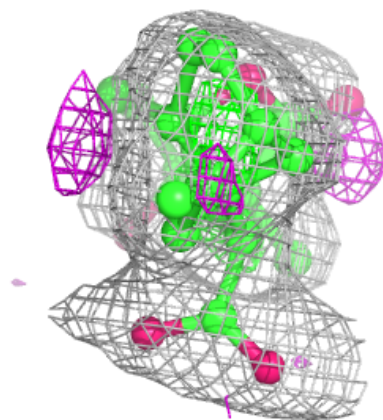
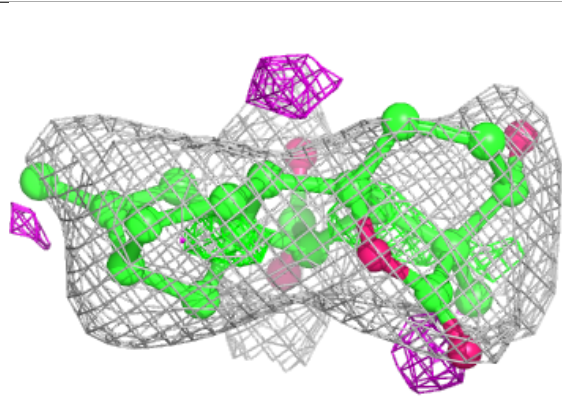
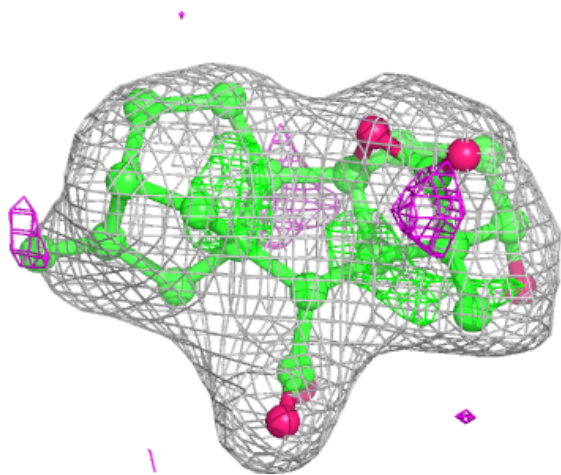
Electron density around GA4 B 401:

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



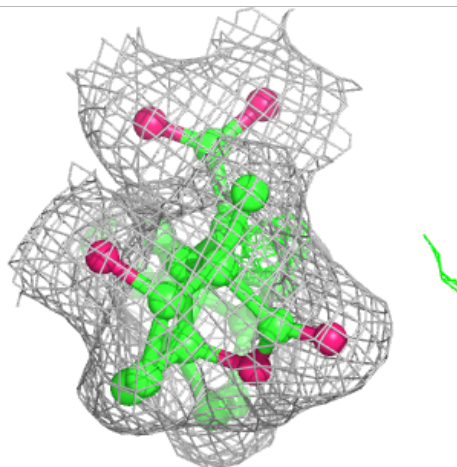
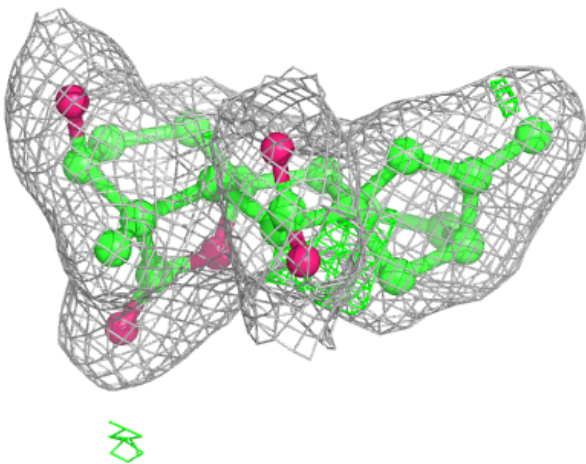
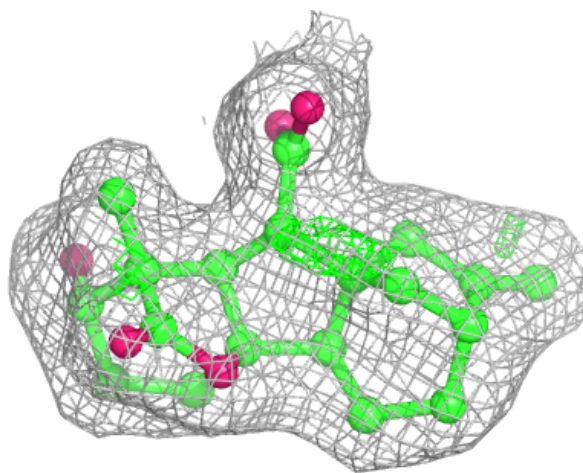
Electron density around GA4 C 402:

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



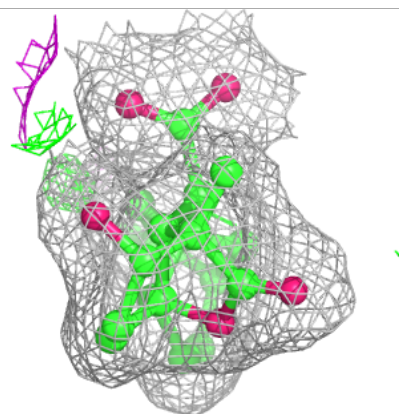
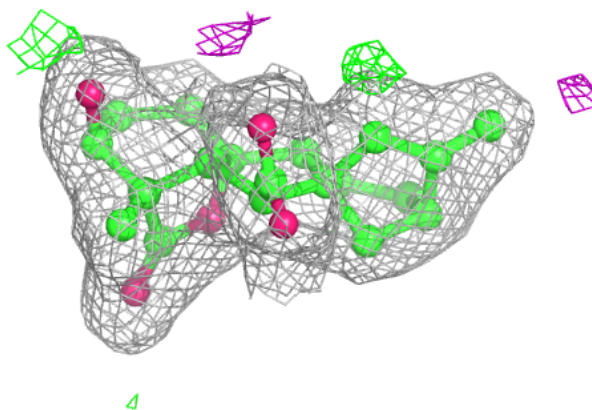
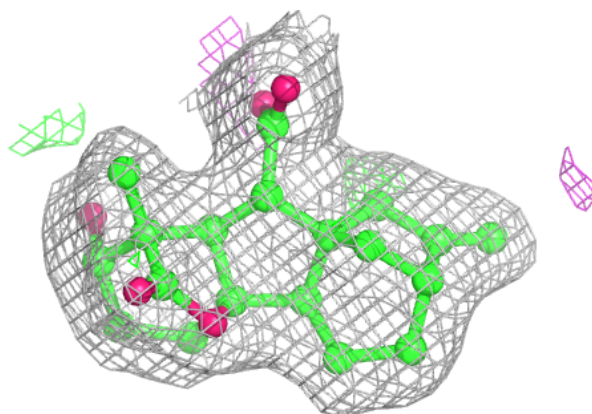
Electron density around GA4 A 402:

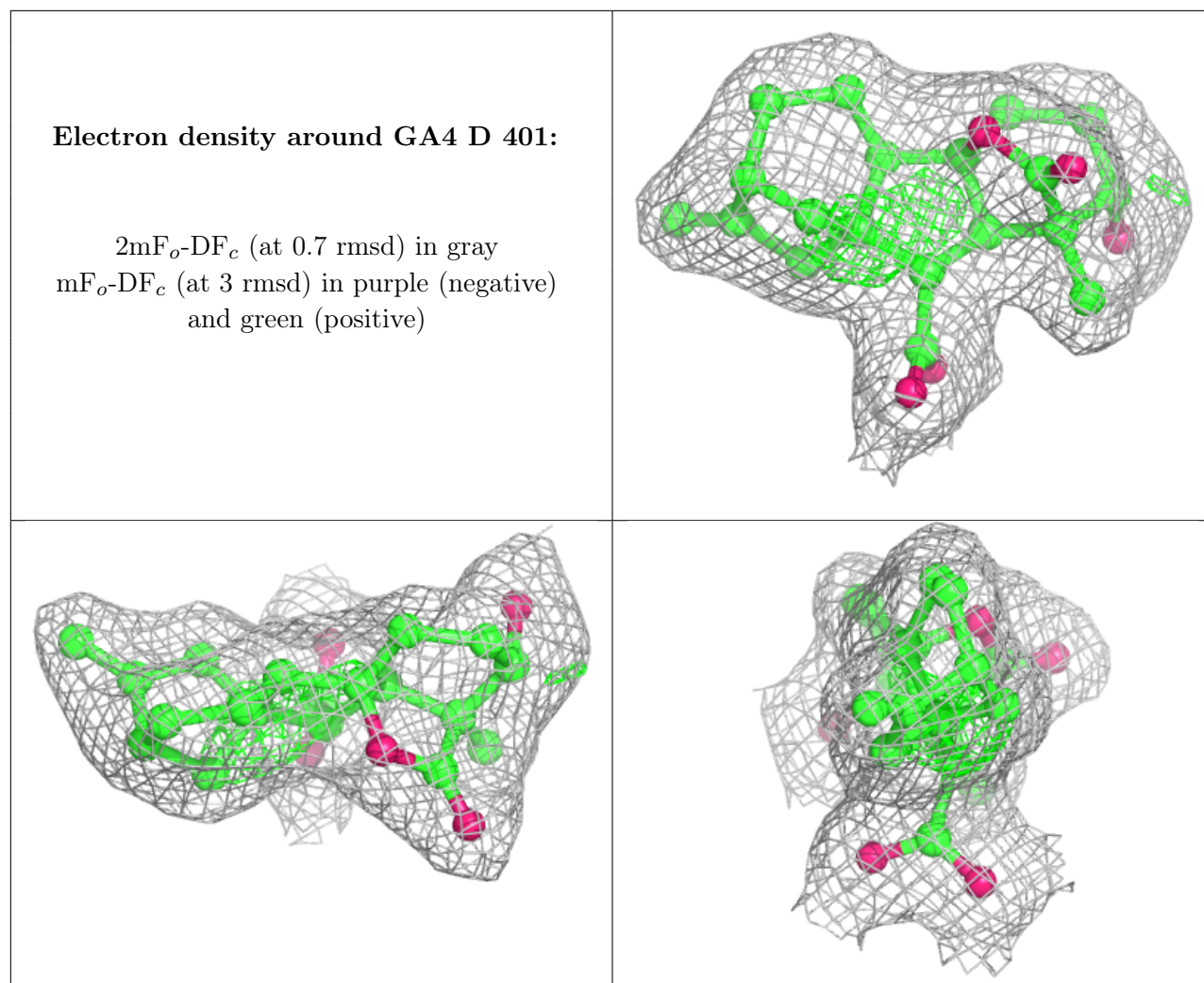
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GA4 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.