



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2022 – 11:12 am BST

PDB ID : 7OV5
Title : Structure of Human Serum Albumin in complex with Aristolochic Acid II at 1.9 Å resolution
Authors : Pomyalov, S.; Sidorenko, V.S.; Grollman, A.P.; Shoham, G.
Deposited on : 2021-06-14
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

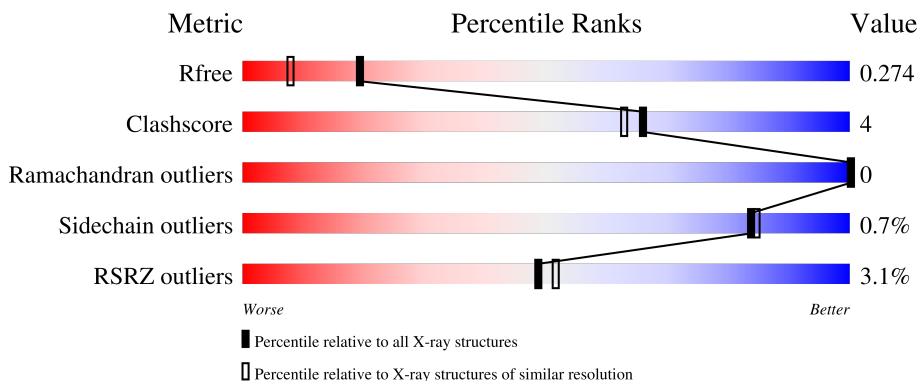
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	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 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	609	 3% 88% 8%
1	B	609	 3% 87% 9%

2 Entry composition [i](#)

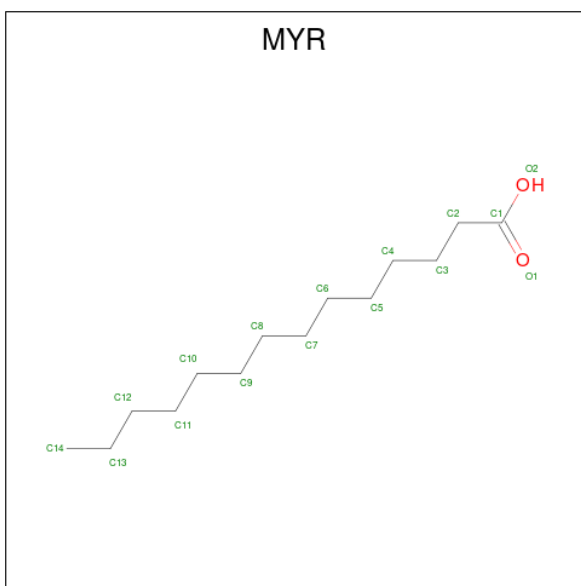
There are 5 unique types of molecules in this entry. The entry contains 10060 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	582	Total 4588	C 2897	N 781	O 869	S 41	0	3	0
1	B	582	Total 4578	C 2890	N 779	O 868	S 41	0	1	0

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 16	C 14	O 2	0	0
2	A	1	Total 16	C 14	O 2	0	0
2	A	1	Total 16	C 14	O 2	0	0
2	A	1	Total 16	C 14	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	B	1	Total	C	O	0	0
			16	14	2		
2	B	1	Total	C	O	0	0
			16	14	2		
2	B	1	Total	C	O	0	0
			16	14	2		
2	B	1	Total	C	O	0	0
			16	14	2		
2	B	1	Total	C	O	0	0
			16	14	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



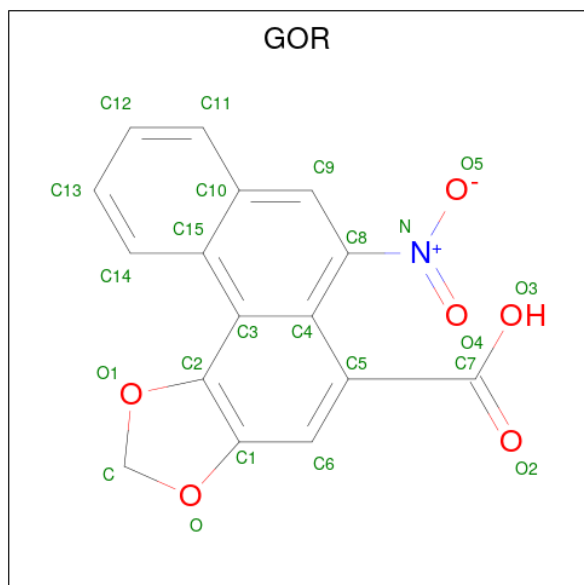
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 4 is 6-nitronaphtho[1,2-e][1,3]benzodioxole-5-carboxylic acid (three-letter code: GOR) (formula: C₁₆H₉NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			23	16	1	6		
4	A	1	Total	C	N	O	0	0
			23	16	1	6		
4	B	1	Total	C	N	O	0	0
			23	16	1	6		
4	B	1	Total	C	N	O	0	0
			23	16	1	6		

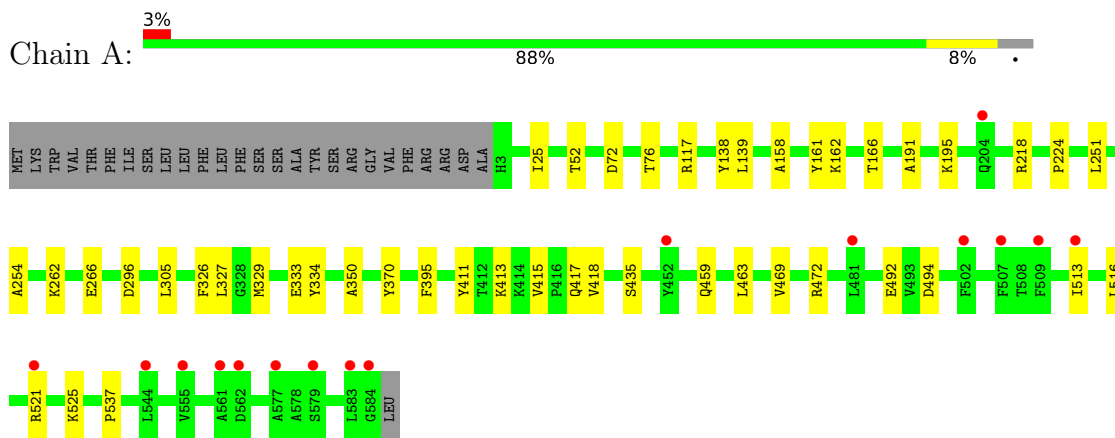
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	307	Total	O	0	0
			307	307		
5	B	287	Total	O	0	0
			287	287		

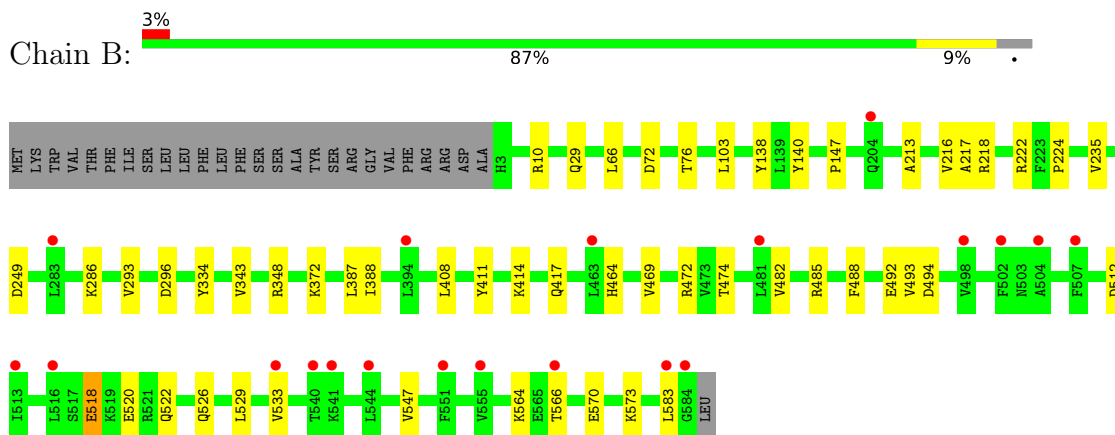
3 Residue-property plots [i](#)

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: Serum albumin



- Molecule 1: Serum albumin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.82Å 38.67Å 180.84Å 90.00° 104.93° 90.00°	Depositor
Resolution (Å)	73.37 – 1.90 73.37 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (73.37-1.90) 98.0 (73.37-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.235 , 0.275 0.234 , 0.274	Depositor DCC
R_{free} test set	4715 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtrriage
Anisotropy	0.358	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10060	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6038e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MYR, EDO, GOR

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	0.37	0/4687	0.48	0/6334
1	B	0.37	0/4668	0.48	0/6309
All	All	0.37	0/9355	0.48	0/12643

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4588	0	4466	31	0
1	B	4578	0	4446	35	0
2	A	96	0	162	11	0
2	B	96	0	162	10	0
3	A	12	0	18	1	0
3	B	4	0	6	1	0
4	A	46	0	0	2	0
4	B	46	0	0	1	0
5	A	307	0	0	1	0
5	B	287	0	0	3	0
All	All	10060	0	9260	74	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 (74) 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:513:ILE:HA	1:A:516:LEU:HD12	1.76	0.68
1:B:518:GLU:OE1	1:B:522:GLN:HG3	1.93	0.67
1:A:52:THR:HB	3:A:607:EDO:H22	1.79	0.63
1:A:326:PHE:HA	1:A:329:MET:HE2	1.83	0.61
1:A:251:LEU:HD21	2:A:602:MYR:H131	1.83	0.60
1:B:417:GLN:HB3	1:B:469:VAL:HG12	1.83	0.60
1:B:411:TYR:HB3	2:B:604:MYR:H112	1.83	0.60
1:A:521:ARG:HG2	1:A:525:LYS:HE2	1.83	0.60
1:A:117:ARG:NH2	2:A:601:MYR:O2	2.32	0.59
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.84	0.59
1:B:488:PHE:HB3	2:B:604:MYR:H71	1.85	0.58
1:A:162:LYS:O	1:A:166:THR:HG23	2.04	0.58
1:B:464:HIS:CD2	1:B:474:THR:HG23	2.39	0.57
1:A:262:LYS:NZ	5:A:711:HOH:O	2.36	0.57
1:A:25:ILE:HD11	1:A:139:LEU:HD11	1.88	0.56
1:B:213:ALA:HB2	2:B:606:MYR:H92	1.87	0.54
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.90	0.54
1:A:158:ALA:HA	2:A:601:MYR:H122	1.92	0.52
1:B:286:LYS:NZ	5:B:708:HOH:O	2.41	0.52
1:B:417:GLN:NE2	1:B:494:ASP:OD2	2.39	0.52
1:A:161:TYR:CD2	2:A:601:MYR:H101	2.44	0.52
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.90	0.52
1:B:222:ARG:HD2	1:B:293:VAL:O	2.13	0.49
1:B:566:THR:O	1:B:570:GLU:HG2	2.12	0.49
1:B:103:LEU:HD11	1:B:249:ASP:HB2	1.95	0.48
2:B:604:MYR:H132	2:B:604:MYR:H101	1.61	0.48
2:B:602:MYR:H92	2:B:602:MYR:H121	1.74	0.47
1:A:161:TYR:CG	2:A:601:MYR:H101	2.48	0.47
1:B:348:ARG:HG3	1:B:482:VAL:HG22	1.97	0.47
1:B:72:ASP:O	1:B:76:THR:HG23	2.14	0.47
1:B:464:HIS:HD2	1:B:474:THR:HG23	1.79	0.47
1:A:417:GLN:NE2	1:A:494:ASP:OD2	2.38	0.47
1:B:29:GLN:HG2	1:B:147:PRO:HA	1.97	0.47
1:A:262:LYS:HE2	1:A:266:GLU:OE1	2.16	0.46
1:A:415:VAL:HG12	1:A:418:VAL:HG23	1.97	0.46
1:A:417:GLN:O	1:A:469:VAL:HG11	2.16	0.46
1:B:547:VAL:HG21	1:B:583:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LYS:HE2	1:A:537:PRO:O	2.17	0.44
1:B:414:LYS:HA	1:B:493:VAL:HA	1.98	0.44
1:A:191:ALA:O	1:A:195:LYS:HG3	2.18	0.43
1:B:573:LYS:HD3	5:B:718:HOH:O	2.18	0.43
1:B:66:LEU:HD23	1:B:66:LEU:HA	1.82	0.43
2:B:601:MYR:H21	2:B:601:MYR:H52	1.85	0.43
1:B:216:VAL:HG22	1:B:235:VAL:HG21	1.99	0.43
1:B:529:LEU:O	1:B:533:VAL:HG23	2.18	0.43
1:A:138:TYR:HB3	2:A:601:MYR:H92	2.01	0.43
1:A:254:ALA:HB1	2:A:602:MYR:H62	2.00	0.43
1:B:217:ALA:HB3	1:B:343:VAL:HG13	2.00	0.43
1:B:372:LYS:HB2	1:B:372:LYS:HE3	1.76	0.43
1:B:485:ARG:HB2	3:B:607:EDO:H12	2.00	0.42
1:B:520:GLU:HG3	5:B:934:HOH:O	2.18	0.42
4:A:610:GOR:O5	4:A:610:GOR:C7	2.67	0.42
1:B:472:ARG:NH2	1:B:492:GLU:O	2.52	0.42
1:A:411:TYR:OH	2:A:604:MYR:O1	2.34	0.42
4:B:609:GOR:C7	4:B:609:GOR:N	2.83	0.42
1:B:512:ASP:OD1	1:B:512:ASP:N	2.50	0.42
1:A:326:PHE:HA	1:A:329:MET:CE	2.48	0.42
1:A:138:TYR:CZ	2:A:601:MYR:H52	2.55	0.41
1:A:459:GLN:O	1:A:463:LEU:HD13	2.20	0.41
1:A:327:LEU:HB3	2:A:606:MYR:H81	2.02	0.41
1:A:350:ALA:HB1	2:A:606:MYR:H72	2.03	0.41
1:B:387:LEU:HD23	1:B:387:LEU:HA	1.90	0.41
1:B:218[B]:ARG:NH2	1:B:222:ARG:HE	2.19	0.41
1:B:408:LEU:HD21	1:B:526:GLN:HB3	2.02	0.41
2:B:601:MYR:H41	2:B:601:MYR:H72	1.45	0.41
1:B:138:TYR:CE1	2:B:601:MYR:H42	2.55	0.41
1:B:10:ARG:HG3	1:B:66:LEU:HD11	2.03	0.41
1:A:72:ASP:O	1:A:76:THR:HG23	2.20	0.41
1:B:518:GLU:OE1	1:B:522:GLN:NE2	2.54	0.41
2:B:601:MYR:H71	2:B:601:MYR:H101	1.84	0.41
4:A:611:GOR:C7	4:A:611:GOR:N	2.84	0.40
1:A:395:PHE:CZ	1:A:435:SER:HA	2.56	0.40
1:A:472:ARG:NH2	1:A:492:GLU:O	2.54	0.40
1:B:388:ILE:HG12	2:B:603:MYR:H81	2.04	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	583/609 (96%)	575 (99%)	8 (1%)	0	100	100
1	B	581/609 (95%)	568 (98%)	13 (2%)	0	100	100
All	All	1164/1218 (96%)	1143 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	496/533 (93%)	492 (99%)	4 (1%)	81	82
1	B	494/533 (93%)	490 (99%)	4 (1%)	81	82
All	All	990/1066 (93%)	982 (99%)	8 (1%)	84	82

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218[A]	ARG
1	A	218[B]	ARG
1	A	334	TYR
1	A	370	TYR
1	B	140	TYR
1	B	334	TYR
1	B	518	GLU
1	B	564	LYS

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

Mol	Chain	Res	Type
1	B	9	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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	$\# Z > 2$
4	GOR	B	608	-	23,26,26	1.19	1 (4%)	28,39,39	0.88	2 (7%)
2	MYR	B	606	-	12,15,15	0.23	0	11,15,15	1.13	0
4	GOR	A	611	-	23,26,26	1.17	2 (8%)	28,39,39	0.81	2 (7%)
2	MYR	B	604	-	12,15,15	0.23	0	11,15,15	1.11	0
2	MYR	B	601	-	12,15,15	0.29	0	11,15,15	0.96	0
3	EDO	A	607	-	3,3,3	0.50	0	2,2,2	0.30	0
3	EDO	B	607	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	A	608	-	3,3,3	0.51	0	2,2,2	0.24	0
3	EDO	A	609	-	3,3,3	0.54	0	2,2,2	0.23	0
2	MYR	A	605	-	12,15,15	0.24	0	11,15,15	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOR	B	609	-	23,26,26	1.24	1 (4%)	28,39,39	0.92	2 (7%)
2	MYR	B	602	-	12,15,15	0.32	0	11,15,15	0.82	0
4	GOR	A	610	-	23,26,26	1.09	1 (4%)	28,39,39	0.92	2 (7%)
2	MYR	A	603	-	12,15,15	0.27	0	11,15,15	0.90	0
2	MYR	B	603	-	12,15,15	0.39	0	11,15,15	0.80	0
2	MYR	A	602	-	12,15,15	0.28	0	11,15,15	0.94	0
2	MYR	A	604	-	12,15,15	0.30	0	11,15,15	0.85	0
2	MYR	A	601	-	12,15,15	0.24	0	11,15,15	0.99	0
2	MYR	A	606	-	12,15,15	0.32	0	11,15,15	0.93	0
2	MYR	B	605	-	12,15,15	0.26	0	11,15,15	0.97	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	GOR	B	608	-	-	1/2/14/14	0/4/4/4
2	MYR	B	606	-	-	4/11/13/13	-
4	GOR	A	611	-	-	2/2/14/14	0/4/4/4
2	MYR	B	604	-	-	5/11/13/13	-
2	MYR	B	601	-	-	7/11/13/13	-
3	EDO	A	607	-	-	1/1/1/1	-
3	EDO	B	607	-	-	0/1/1/1	-
3	EDO	A	608	-	-	0/1/1/1	-
3	EDO	A	609	-	-	0/1/1/1	-
2	MYR	A	605	-	-	7/11/13/13	-
4	GOR	B	609	-	-	2/2/14/14	0/4/4/4
2	MYR	B	602	-	-	4/11/13/13	-
4	GOR	A	610	-	-	1/2/14/14	0/4/4/4
2	MYR	A	603	-	-	5/11/13/13	-
2	MYR	B	603	-	-	5/11/13/13	-
2	MYR	A	602	-	-	3/11/13/13	-
2	MYR	A	604	-	-	8/11/13/13	-
2	MYR	A	601	-	-	5/11/13/13	-
2	MYR	A	606	-	-	3/11/13/13	-
2	MYR	B	605	-	-	6/11/13/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	609	GOR	C5-C7	5.26	1.52	1.47
4	B	608	GOR	C5-C7	4.90	1.52	1.47
4	A	611	GOR	C5-C7	4.59	1.51	1.47
4	A	610	GOR	C5-C7	4.42	1.51	1.47
4	A	611	GOR	C3-C4	2.21	1.46	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	608	GOR	C8-C4-C3	-3.30	116.44	118.69
4	A	610	GOR	C8-C4-C3	-3.23	116.48	118.69
4	B	609	GOR	C8-C4-C3	-2.83	116.75	118.69
4	A	611	GOR	C8-C4-C3	-2.68	116.86	118.69
4	B	608	GOR	C6-C5-C4	2.54	120.89	117.53
4	A	611	GOR	C6-C5-C4	2.50	120.84	117.53
4	B	609	GOR	C6-C5-C4	2.43	120.73	117.53
4	A	610	GOR	C6-C5-C4	2.34	120.62	117.53

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	MYR	C1-C2-C3-C4
2	A	604	MYR	C1-C2-C3-C4
2	A	605	MYR	C1-C2-C3-C4
2	A	606	MYR	C1-C2-C3-C4
2	B	605	MYR	C1-C2-C3-C4
2	B	606	MYR	C1-C2-C3-C4
4	A	611	GOR	C4-C8-N-O4
4	A	611	GOR	C9-C8-N-O4
4	B	609	GOR	C4-C8-N-O4
4	B	609	GOR	C9-C8-N-O4
2	A	601	MYR	C10-C11-C12-C13
2	B	601	MYR	C4-C5-C6-C7
2	B	601	MYR	C7-C8-C9-C10
4	A	610	GOR	C9-C8-N-O4
2	A	604	MYR	C3-C4-C5-C6
2	A	604	MYR	C4-C5-C6-C7
2	A	601	MYR	C5-C6-C7-C8
2	B	601	MYR	C5-C6-C7-C8
2	B	603	MYR	C10-C11-C12-C13
2	A	606	MYR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	B	605	MYR	C11-C10-C9-C8
2	B	604	MYR	C5-C6-C7-C8
2	A	606	MYR	C5-C6-C7-C8
2	A	604	MYR	C11-C10-C9-C8
2	A	604	MYR	C7-C8-C9-C10
2	A	604	MYR	C6-C7-C8-C9
2	B	603	MYR	C11-C10-C9-C8
2	B	601	MYR	C3-C4-C5-C6
2	B	602	MYR	C2-C3-C4-C5
2	A	605	MYR	C2-C3-C4-C5
2	B	605	MYR	C5-C6-C7-C8
2	B	606	MYR	C6-C7-C8-C9
2	A	603	MYR	C7-C8-C9-C10
2	B	604	MYR	C4-C5-C6-C7
2	A	605	MYR	C6-C7-C8-C9
2	A	602	MYR	C3-C4-C5-C6
2	A	602	MYR	C9-C10-C11-C12
2	A	601	MYR	C3-C4-C5-C6
2	B	601	MYR	C2-C3-C4-C5
2	A	603	MYR	C3-C4-C5-C6
2	B	604	MYR	C2-C3-C4-C5
2	A	601	MYR	C4-C5-C6-C7
4	B	608	GOR	C9-C8-N-O4
2	A	602	MYR	C5-C6-C7-C8
2	B	602	MYR	C10-C11-C12-C13
2	A	605	MYR	C9-C10-C11-C12
2	B	605	MYR	C7-C8-C9-C10
2	A	604	MYR	C2-C3-C4-C5
2	A	605	MYR	C10-C11-C12-C13
2	B	606	MYR	C3-C4-C5-C6
2	B	604	MYR	C6-C7-C8-C9
2	B	601	MYR	C1-C2-C3-C4
2	A	605	MYR	C5-C6-C7-C8
2	B	603	MYR	C3-C4-C5-C6
2	A	603	MYR	C5-C6-C7-C8
2	B	605	MYR	C9-C10-C11-C12
2	B	606	MYR	C9-C10-C11-C12
2	A	603	MYR	C4-C5-C6-C7
2	B	604	MYR	C10-C11-C12-C13
2	B	603	MYR	C6-C7-C8-C9
2	B	605	MYR	C6-C7-C8-C9
3	A	607	EDO	O1-C1-C2-O2

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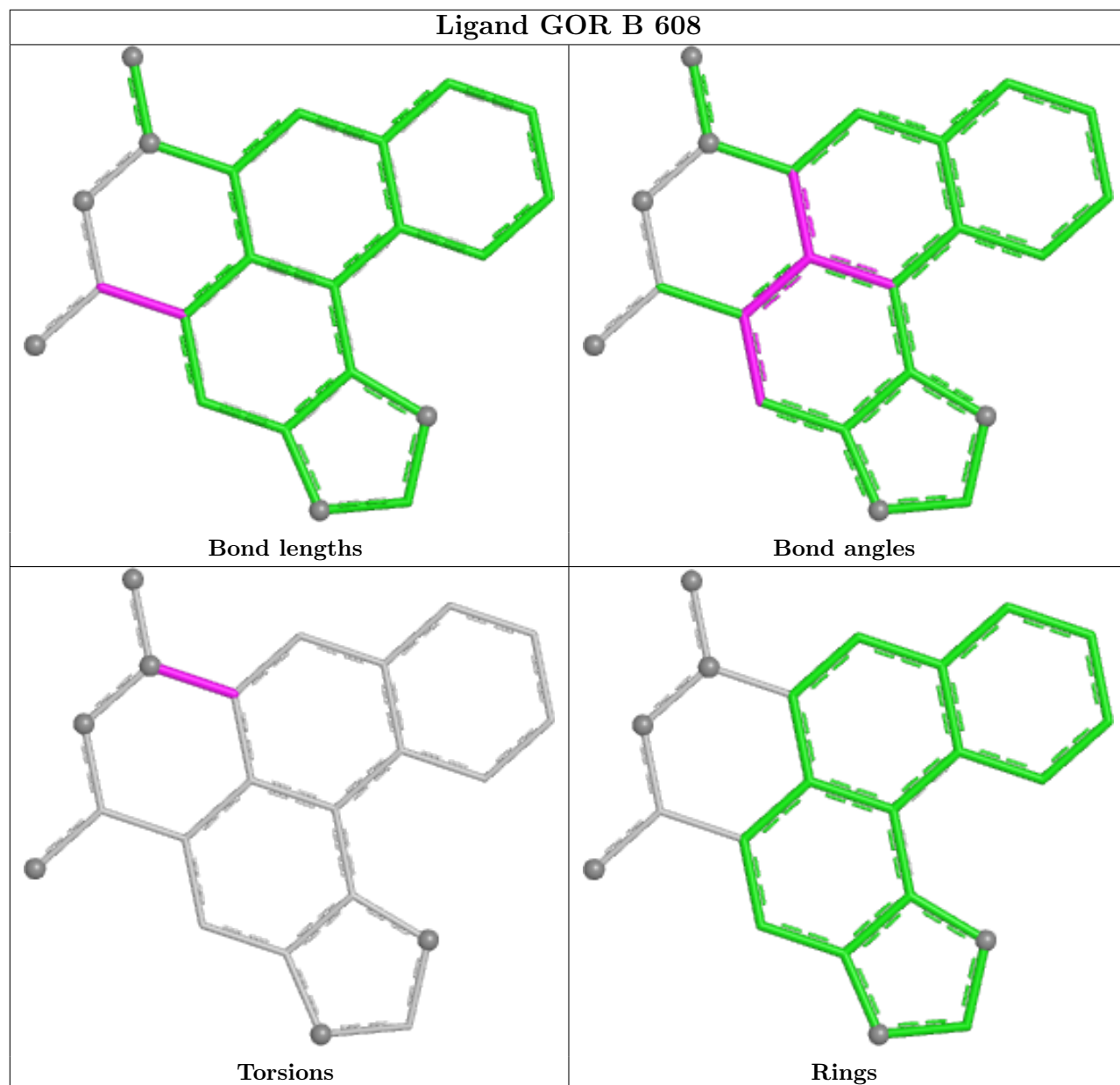
Mol	Chain	Res	Type	Atoms
2	A	604	MYR	C9-C10-C11-C12
2	B	602	MYR	C11-C12-C13-C14
2	B	601	MYR	C6-C7-C8-C9
2	A	603	MYR	C10-C11-C12-C13
2	B	603	MYR	C2-C3-C4-C5
2	B	602	MYR	C9-C10-C11-C12
2	A	605	MYR	C11-C10-C9-C8

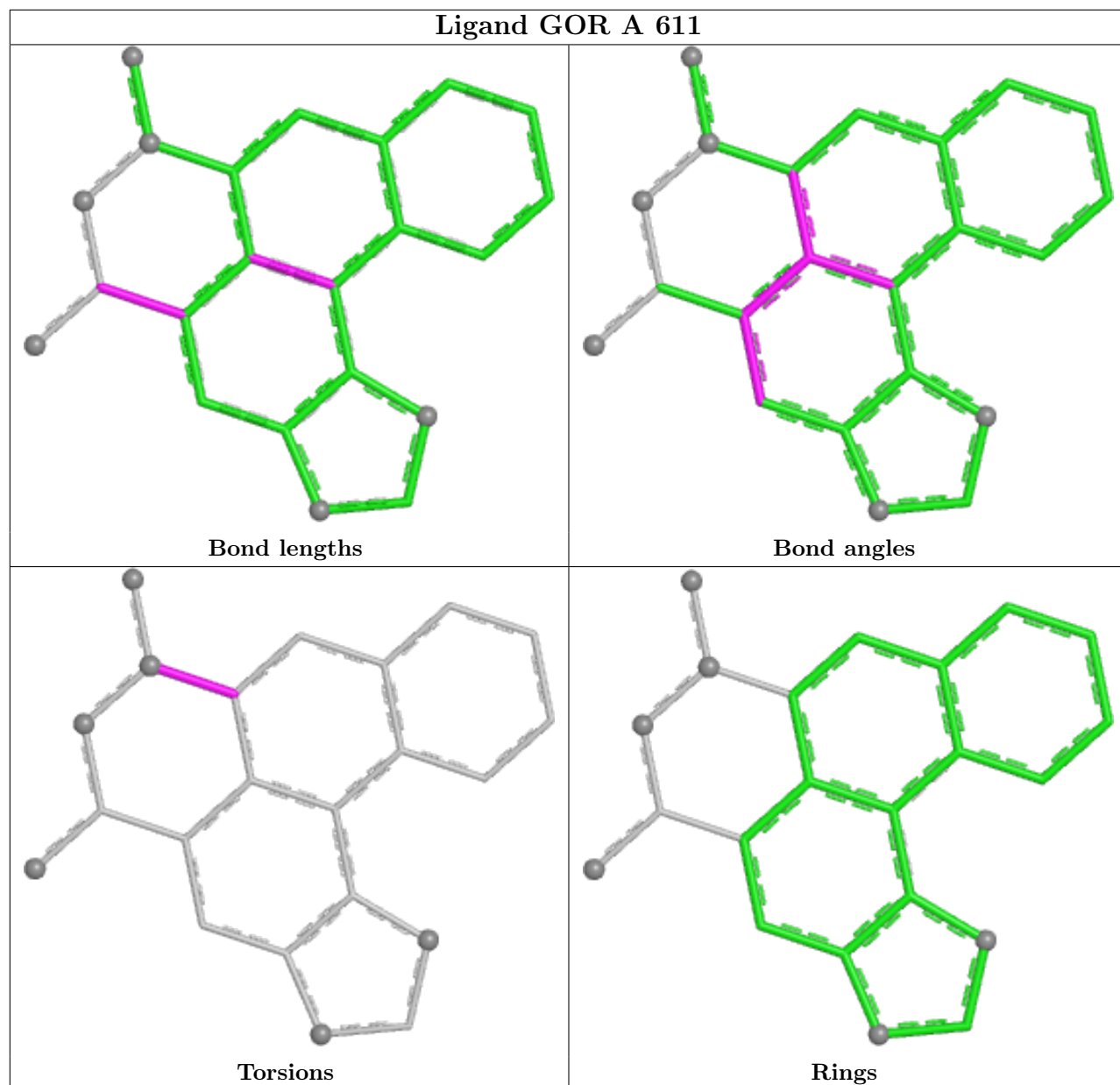
There are no ring outliers.

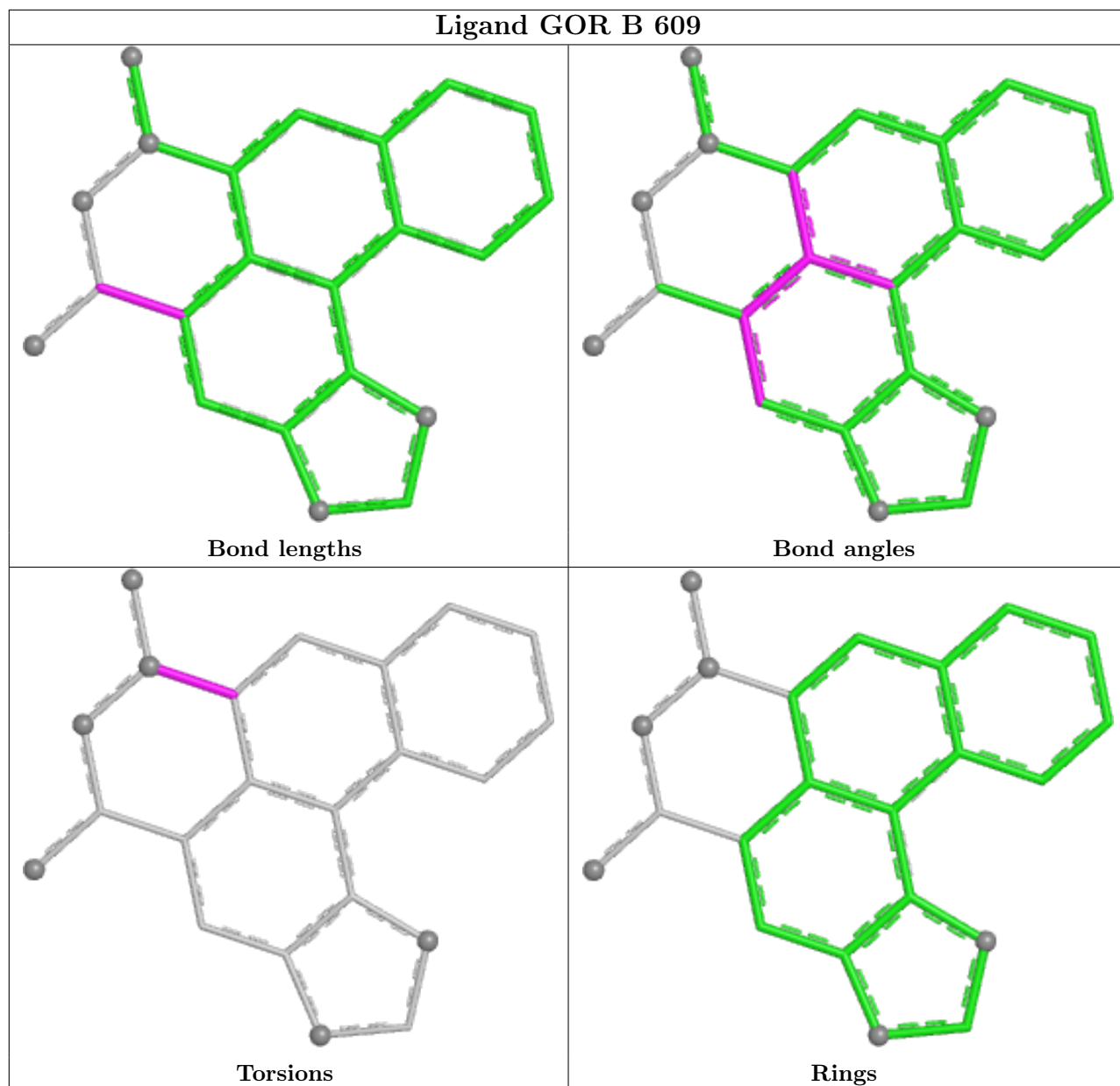
14 monomers are involved in 26 short contacts:

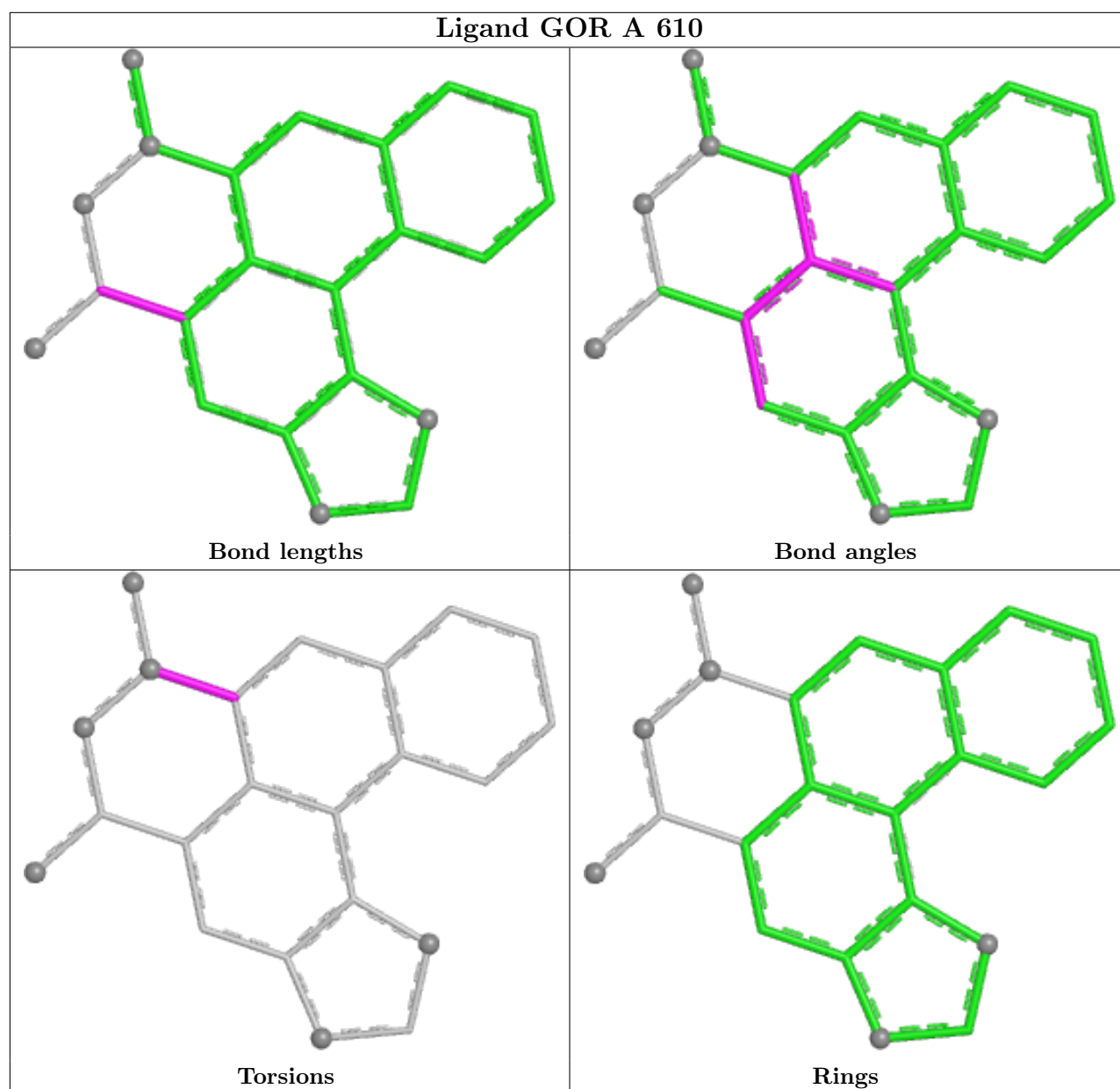
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	606	MYR	1	0
4	A	611	GOR	1	0
2	B	604	MYR	3	0
2	B	601	MYR	4	0
3	A	607	EDO	1	0
3	B	607	EDO	1	0
4	B	609	GOR	1	0
2	B	602	MYR	1	0
4	A	610	GOR	1	0
2	B	603	MYR	1	0
2	A	602	MYR	2	0
2	A	604	MYR	1	0
2	A	601	MYR	6	0
2	A	606	MYR	2	0

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	582/609 (95%)	0.24	16 (2%) 54 57	25, 39, 58, 84	0
1	B	582/609 (95%)	0.32	20 (3%) 45 48	24, 40, 62, 84	0
All	All	1164/1218 (95%)	0.28	36 (3%) 49 51	24, 39, 60, 84	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	502	PHE	5.0
1	A	583	LEU	4.5
1	A	481	LEU	4.3
1	A	509	PHE	4.0
1	B	507	PHE	3.9
1	B	555	VAL	3.9
1	A	561	ALA	3.2
1	A	584	GLY	3.2
1	B	504	ALA	3.1
1	B	498	VAL	3.0
1	A	502	PHE	3.0
1	B	513	ILE	2.9
1	B	584	GLY	2.8
1	B	583	LEU	2.8
1	A	579	SER	2.6
1	B	481	LEU	2.6
1	B	516	LEU	2.5
1	B	283	LEU	2.5
1	A	204	GLN	2.4
1	B	566	THR	2.4
1	B	463	LEU	2.4
1	B	540	THR	2.3
1	A	555	VAL	2.3
1	A	577	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	541	LYS	2.2
1	B	204	GLN	2.2
1	A	507	PHE	2.2
1	A	562	ASP	2.2
1	A	452	TYR	2.2
1	B	544	LEU	2.1
1	A	513	ILE	2.1
1	A	544	LEU	2.1
1	A	521	ARG	2.1
1	B	533	VAL	2.1
1	B	551	PHE	2.1
1	B	394	LEU	2.1

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
2	MYR	A	601	16/16	0.69	0.26	33,40,46,47	16
2	MYR	A	604	16/16	0.73	0.28	40,46,57,60	16
2	MYR	B	601	16/16	0.74	0.21	27,39,50,50	16
2	MYR	B	605	16/16	0.74	0.26	43,49,60,61	0
2	MYR	B	604	16/16	0.77	0.26	40,44,49,55	0
2	MYR	A	606	16/16	0.77	0.29	33,37,56,57	16
4	GOR	B	609	23/23	0.77	0.19	32,41,51,56	23
2	MYR	B	606	16/16	0.78	0.27	29,37,63,67	16
2	MYR	A	605	16/16	0.79	0.27	42,46,58,62	0
4	GOR	A	611	23/23	0.80	0.22	35,39,57,58	23
2	MYR	B	602	16/16	0.82	0.20	33,39,45,46	16

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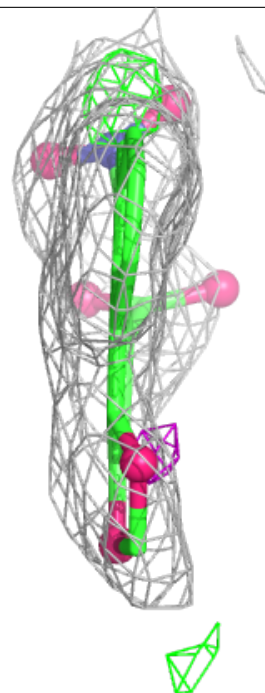
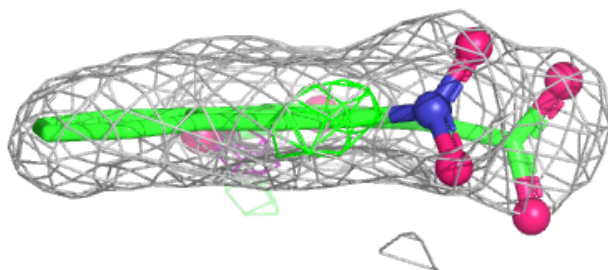
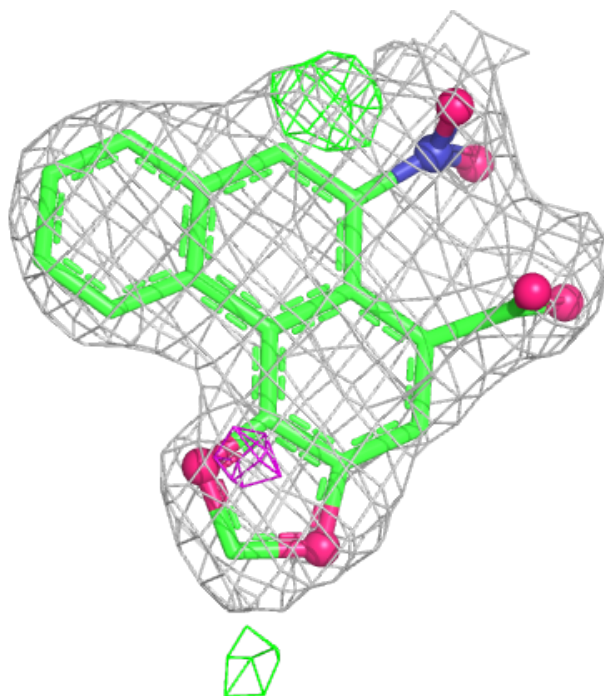
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MYR	A	602	16/16	0.83	0.21	34,40,47,48	0
3	EDO	A	608	4/4	0.87	0.28	42,49,51,59	0
3	EDO	B	607	4/4	0.87	0.16	40,41,44,44	0
4	GOR	A	610	23/23	0.89	0.12	29,33,39,44	0
3	EDO	A	609	4/4	0.89	0.13	35,35,40,41	0
3	EDO	A	607	4/4	0.89	0.24	34,39,46,46	0
4	GOR	B	608	23/23	0.90	0.12	28,35,40,42	0
2	MYR	B	603	16/16	0.93	0.15	31,37,51,52	0
2	MYR	A	603	16/16	0.93	0.16	29,39,51,53	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.

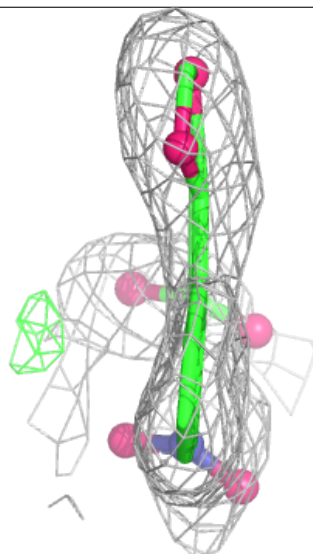
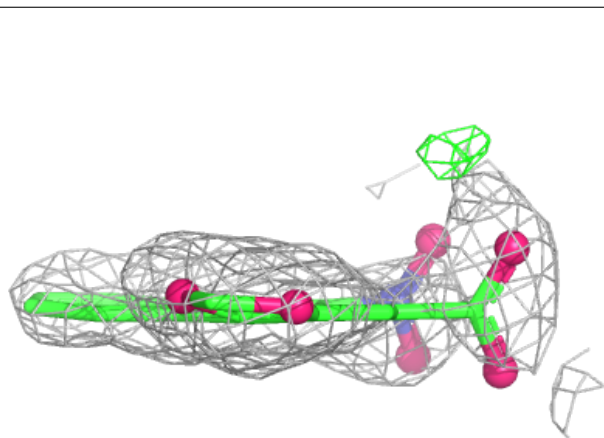
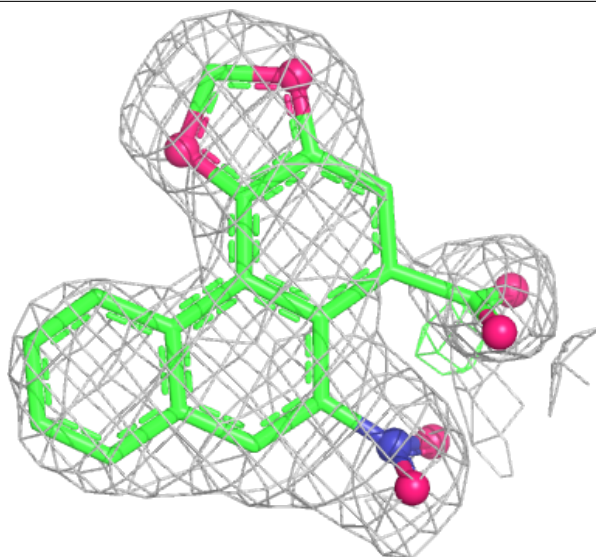
Electron density around GOR B 609:

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



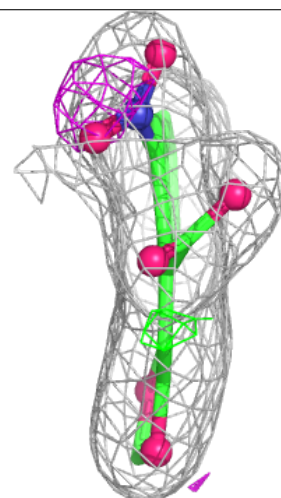
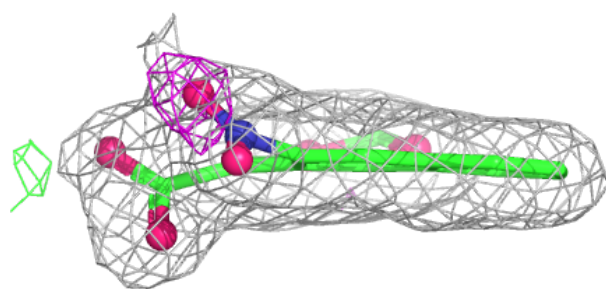
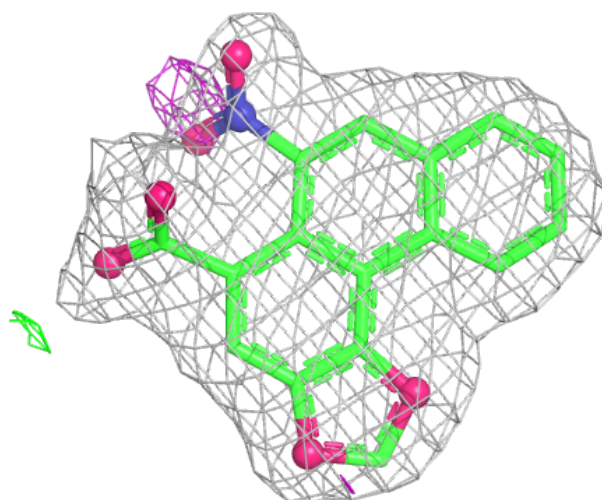
Electron density around GOR A 611:

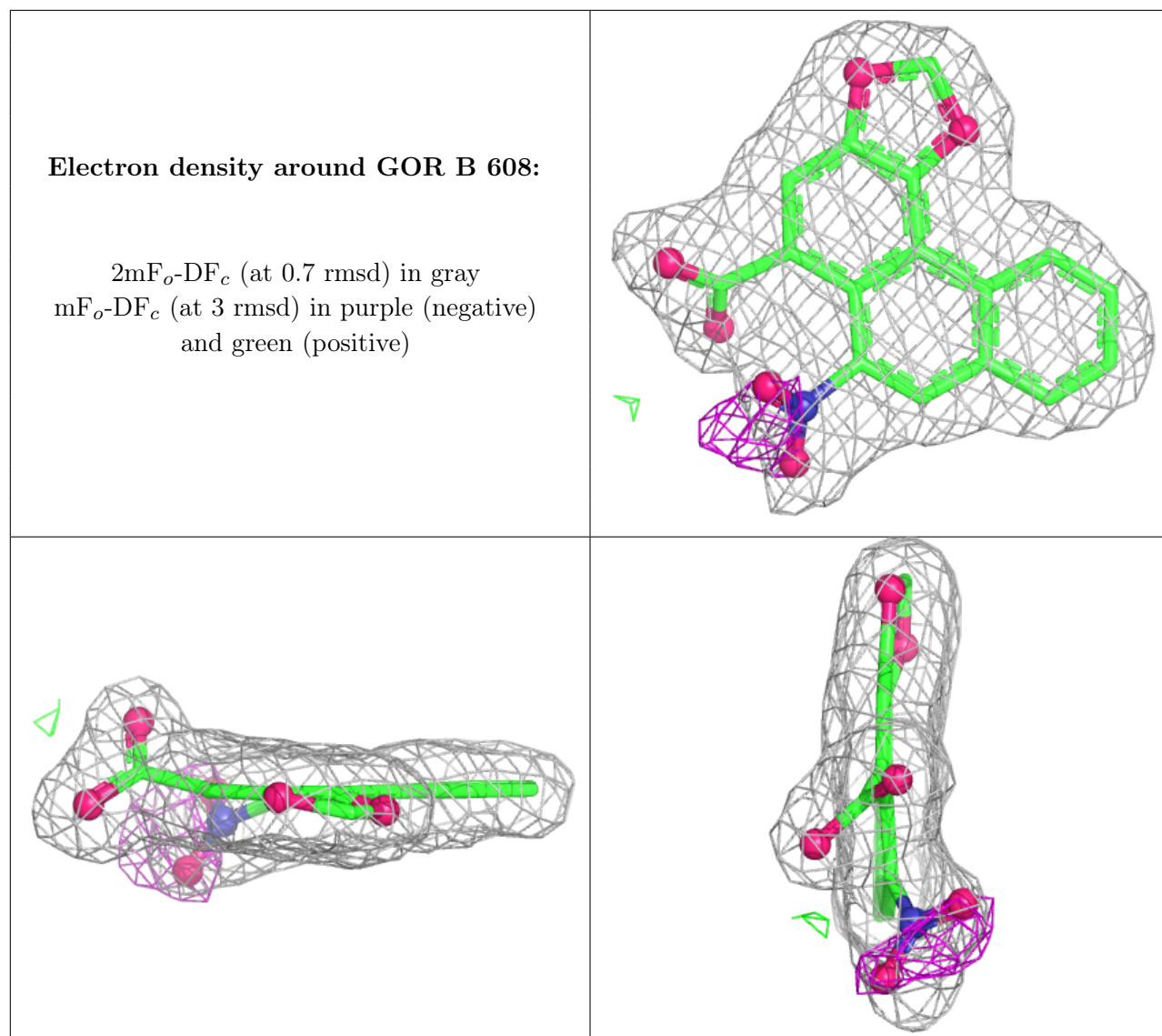
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GOR A 610:

$2mF_o-DF_c$ (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.