



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:20 AM UTC

PDB ID : 8RCO / pdb_00008rco
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 : 2023-12-06
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

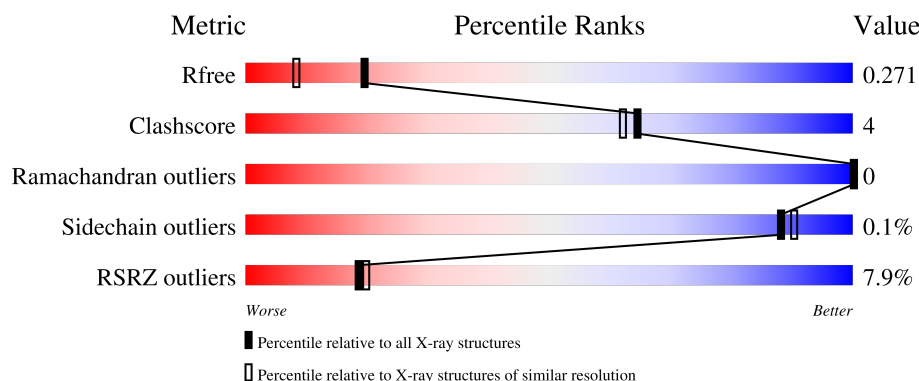
1 Overall quality at a glance

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	609	6% 88% 8%
1	B	609	9% 88% 8%

2 Entry composition [i](#)

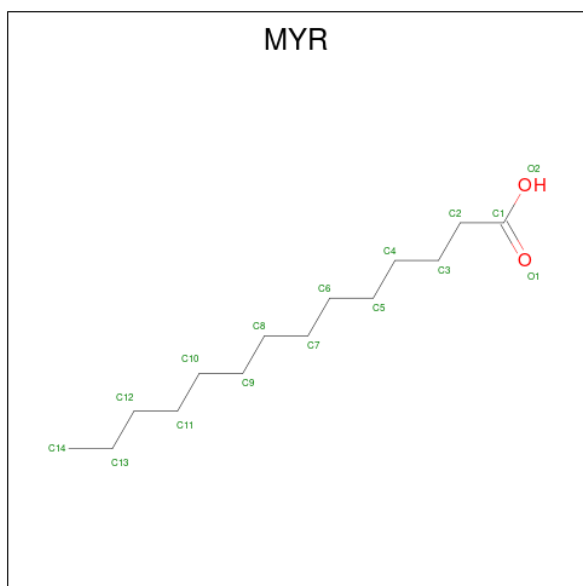
There are 5 unique types of molecules in this entry. The entry contains 19340 atoms, of which 9287 are hydrogens and 0 are deuteriums.

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
1	A	582	Total	C	H	N	O	S	0	3	0
			9040	2891	4459	781	868	41			
1	B	582	Total	C	H	N	O	S	0	2	0
			9026	2890	4448	779	868	41			

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



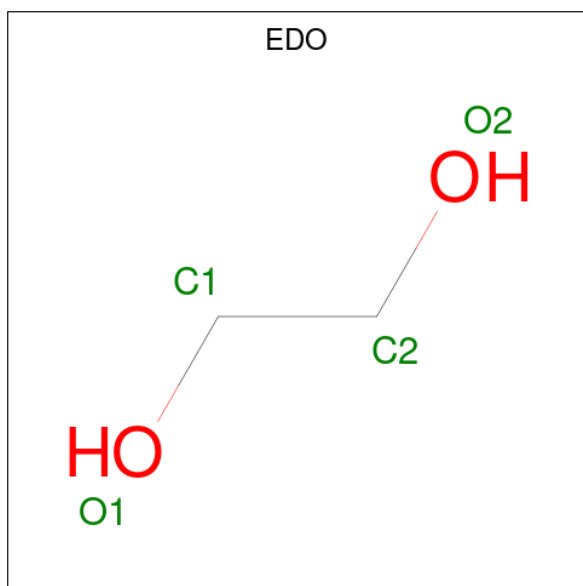
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			43	14	27	2		
2	A	1	Total	C	H	O	0	0
			43	14	27	2		
2	A	1	Total	C	H	O	0	0
			43	14	27	2		
2	A	1	Total	C	H	O	0	0
			43	14	27	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			43	14	27	2		
2	A	1	Total	C	H	O	0	0
			43	14	27	2		
2	B	1	Total	C	H	O	0	0
			43	14	27	2		
2	B	1	Total	C	H	O	0	0
			43	14	27	2		
2	B	1	Total	C	H	O	0	0
			43	14	27	2		
2	B	1	Total	C	H	O	0	0
			43	14	27	2		
2	B	1	Total	C	H	O	0	0
			43	14	27	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



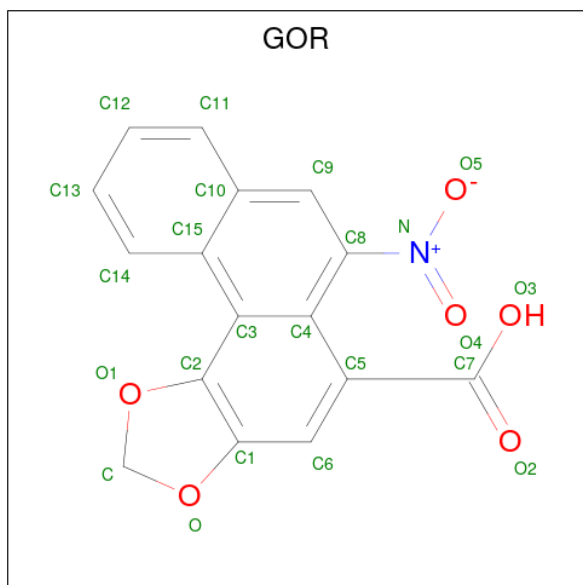
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			10	2	6	2		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			31	16	8	1	6		
4	A	1	Total	C	H	N	O	0	0
			31	16	8	1	6		
4	B	1	Total	C	H	N	O	0	0
			31	16	8	1	6		
4	B	1	Total	C	H	N	O	0	0
			31	16	8	1	6		

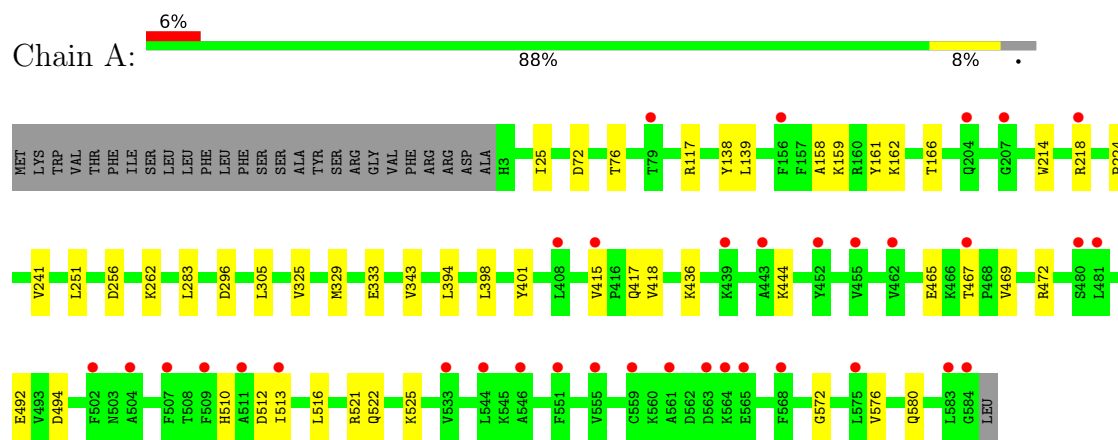
- Molecule 5 is water.

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

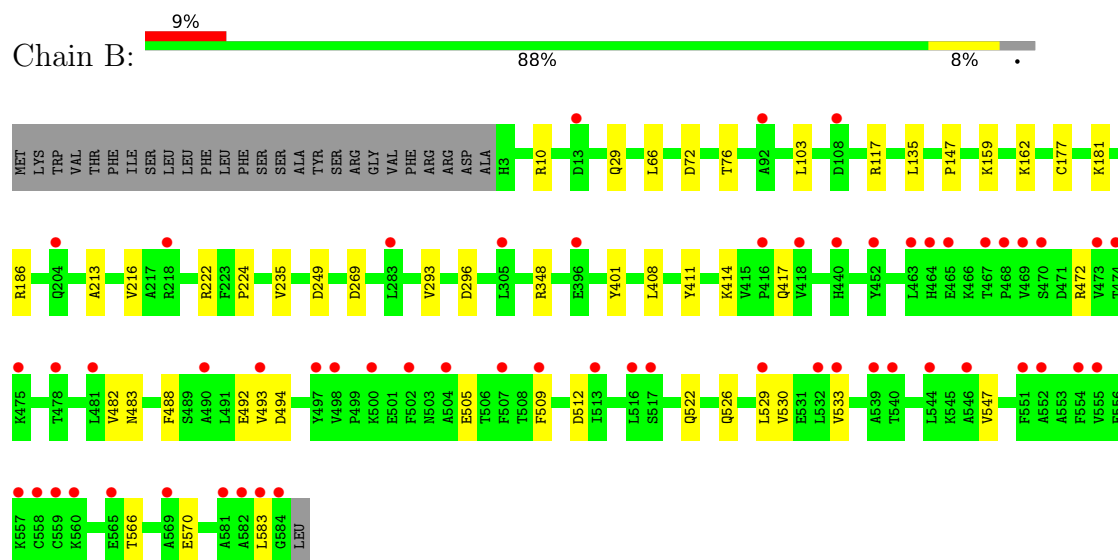
3 Residue-property plots

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) 97.9 (73.37-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.230 , 0.271 0.231 , 0.271	Depositor DCC
R_{free} test set	4770 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19340	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage'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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GOR, MYR, EDO

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	0.18	0/4679	0.30	0/6323
1	B	0.18	0/4676	0.29	0/6320
All	All	0.18	0/9355	0.29	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	4581	4459	4457	38	0
1	B	4578	4448	4436	31	0
2	A	96	162	162	5	0
2	B	96	162	162	4	0
3	A	12	18	18	0	0
3	B	4	6	6	0	0
4	A	46	16	0	2	0
4	B	46	16	0	3	0
5	A	307	0	0	4	0
5	B	287	0	0	3	0
All	All	10053	9287	9241	73	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 (73) 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:444:LYS:NZ	5:A:701:HOH:O	1.99	0.95
1:B:483:ASN:OD1	5:B:701:HOH:O	2.07	0.71
1:B:269:ASP:OD1	5:B:702:HOH:O	2.11	0.67
1:A:576:VAL:HG12	1:A:580:GLN:HE21	1.58	0.67
1:A:444:LYS:HA	1:A:444:LYS:HE2	1.78	0.64
1:A:162:LYS:O	1:A:166:THR:HG23	1.98	0.63
1:A:117:ARG:NH2	2:A:601:MYR:O2	2.33	0.62
1:B:186:ARG:NH2	4:B:609:GOR:O3	2.32	0.62
1:A:251:LEU:HD21	2:A:602:MYR:H131	1.85	0.59
1:B:159:LYS:NZ	5:B:705:HOH:O	2.35	0.59
1:A:415:VAL:HG12	1:A:418:VAL:HG23	1.84	0.58
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.86	0.56
1:A:513:ILE:HA	1:A:516:LEU:HD12	1.89	0.54
1:A:262:LYS:NZ	5:A:716:HOH:O	2.40	0.53
1:A:25:ILE:HD11	1:A:139:LEU:HD11	1.92	0.52
1:A:325:VAL:O	1:A:329:MET:HG3	2.11	0.50
1:A:512:ASP:OD2	1:A:512:ASP:N	2.44	0.50
1:B:411:TYR:HB3	2:B:604:MYR:H112	1.93	0.50
1:A:521:ARG:HG2	1:A:525:LYS:HE2	1.92	0.50
1:A:415:VAL:CG1	1:A:418:VAL:HG23	2.42	0.49
1:B:117:ARG:HE	2:B:601:MYR:H21	1.77	0.49
1:B:417:GLN:NE2	1:B:494:ASP:OD2	2.41	0.49
1:B:488:PHE:HB3	2:B:604:MYR:H71	1.93	0.49
1:A:467:THR:HG23	1:A:467:THR:O	2.14	0.48
1:B:505:GLU:OE2	1:B:505:GLU:O	2.32	0.48
1:A:444:LYS:HA	1:A:444:LYS:CE	2.43	0.47
1:B:348:ARG:HG3	1:B:482:VAL:HG22	1.96	0.47
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.95	0.47
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.97	0.47
4:B:609:GOR:C7	4:B:609:GOR:N	2.78	0.47
4:A:611:GOR:C7	4:A:611:GOR:N	2.77	0.47
1:B:213:ALA:HB2	2:B:606:MYR:H92	1.95	0.47
1:B:72:ASP:O	1:B:76:THR:HG23	2.15	0.46
1:A:401:TYR:CE1	1:A:522:GLN:HG2	2.50	0.46
1:B:401:TYR:CE1	1:B:522:GLN:HG2	2.51	0.46
1:A:158:ALA:HA	2:A:601:MYR:H122	1.98	0.45
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:HIS:HB2	1:A:512:ASP:OD2	2.16	0.45
1:B:216:VAL:HG22	1:B:235:VAL:HG21	1.98	0.45
4:A:610:GOR:O5	4:A:610:GOR:C7	2.65	0.45
1:B:529:LEU:O	1:B:533:VAL:HG23	2.17	0.45
1:B:222:ARG:HD2	1:B:293:VAL:O	2.17	0.45
1:B:547:VAL:HG21	1:B:583:LEU:HD21	1.99	0.44
1:B:408:LEU:HD22	1:B:530:VAL:CG2	2.47	0.44
1:B:512:ASP:OD1	1:B:512:ASP:N	2.48	0.43
1:B:29:GLN:HG2	1:B:147:PRO:HA	2.01	0.43
1:B:472:ARG:NH2	1:B:492:GLU:O	2.52	0.42
1:A:417:GLN:NE2	1:A:494:ASP:OD2	2.43	0.42
4:B:608:GOR:O4	4:B:608:GOR:C7	2.67	0.42
1:A:417:GLN:O	1:A:469:VAL:HG11	2.19	0.42
1:B:566:THR:O	1:B:570:GLU:HG2	2.19	0.42
1:A:159:LYS:NZ	5:A:732:HOH:O	2.53	0.42
1:A:516:LEU:O	1:A:521:ARG:NH2	2.52	0.42
1:B:177:CYS:SG	1:B:181:LYS:NZ	2.92	0.41
1:B:509:PHE:CD1	1:B:509:PHE:N	2.88	0.41
1:B:408:LEU:HD22	1:B:530:VAL:HG22	2.01	0.41
1:A:161:TYR:CD2	2:A:601:MYR:H101	2.55	0.41
1:A:444:LYS:CE	5:A:701:HOH:O	2.61	0.41
1:B:10:ARG:HG3	1:B:66:LEU:HD11	2.02	0.41
1:B:103:LEU:HD11	1:B:249:ASP:HB2	2.03	0.41
1:A:283:LEU:C	1:A:283:LEU:HD13	2.46	0.41
1:B:135:LEU:CD1	1:B:162:LYS:HE3	2.51	0.41
1:B:414:LYS:HA	1:B:493:VAL:HA	2.02	0.41
1:A:72:ASP:O	1:A:76:THR:HG23	2.20	0.41
1:A:436:LYS:HD2	1:A:436:LYS:C	2.46	0.40
1:A:465:GLU:OE1	1:A:465:GLU:HA	2.20	0.40
1:A:572:GLY:O	1:A:576:VAL:HG23	2.21	0.40
1:A:138:TYR:HB3	2:A:601:MYR:H92	2.03	0.40
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.56	0.40
1:A:241:VAL:HG22	1:A:256:ASP:HB3	2.03	0.40
1:A:394:LEU:HD11	1:A:398:LEU:HD11	2.04	0.40
1:A:417:GLN:HB3	1:A:469:VAL:CG1	2.52	0.40
1:A:472:ARG:NH2	1:A:492:GLU:O	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	583/609 (96%)	573 (98%)	10 (2%)	0	100	100
1	B	582/609 (96%)	570 (98%)	12 (2%)	0	100	100
All	All	1165/1218 (96%)	1143 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	495/533 (93%)	493 (100%)	2 (0%)	84	87
1	B	495/533 (93%)	495 (100%)	0	100	100
All	All	990/1066 (93%)	988 (100%)	2 (0%)	88	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218[A]	ARG
1	A	218[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN

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Mol	Chain	Res	Type
1	A	61	ASN
1	A	288	HIS
1	A	580	GLN
1	B	242	HIS
1	B	464	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 oligosaccharides 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	$\# Z > 2$
2	MYR	A	605	-	15,15,15	0.64	0	15,15,15	1.11	0
2	MYR	A	606	-	15,15,15	0.61	0	15,15,15	1.11	0
4	GOR	B	609	-	26,26,26	0.68	0	28,39,39	0.74	1 (3%)
2	MYR	A	603	-	15,15,15	0.64	0	15,15,15	1.01	0
2	MYR	A	601	-	15,15,15	0.64	0	15,15,15	1.01	0
2	MYR	B	601	-	15,15,15	0.62	0	15,15,15	0.94	0
4	GOR	A	611	-	26,26,26	0.68	0	28,39,39	0.77	1 (3%)
4	GOR	A	610	-	26,26,26	0.69	0	28,39,39	0.81	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	609	-	3,3,3	0.47	0	2,2,2	0.33	0
2	MYR	B	605	-	15,15,15	0.61	0	15,15,15	1.19	1 (6%)
2	MYR	B	604	-	15,15,15	0.64	0	15,15,15	1.09	0
2	MYR	B	602	-	15,15,15	0.66	0	15,15,15	1.00	0
2	MYR	A	604	-	15,15,15	0.64	0	15,15,15	1.06	1 (6%)
3	EDO	B	607	-	3,3,3	0.45	0	2,2,2	0.30	0
2	MYR	B	603	-	15,15,15	0.65	0	15,15,15	1.03	1 (6%)
2	MYR	A	602	-	15,15,15	0.61	0	15,15,15	1.10	0
4	GOR	B	608	-	26,26,26	0.69	0	28,39,39	0.77	1 (3%)
3	EDO	A	608	-	3,3,3	0.46	0	2,2,2	0.38	0
3	EDO	A	607	-	3,3,3	0.46	0	2,2,2	0.37	0
2	MYR	B	606	-	15,15,15	0.59	0	15,15,15	1.16	1 (6%)

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	MYR	A	605	-	-	6/13/13/13	-
2	MYR	A	606	-	-	6/13/13/13	-
4	GOR	B	609	-	-	6/6/14/14	0/4/4/4
2	MYR	A	603	-	-	7/13/13/13	-
2	MYR	A	601	-	-	5/13/13/13	-
2	MYR	B	601	-	-	6/13/13/13	-
4	GOR	A	611	-	-	6/6/14/14	0/4/4/4
4	GOR	A	610	-	-	2/6/14/14	0/4/4/4
3	EDO	A	609	-	-	0/1/1/1	-
2	MYR	B	605	-	-	7/13/13/13	-
2	MYR	B	604	-	-	5/13/13/13	-
2	MYR	B	602	-	-	3/13/13/13	-
2	MYR	A	604	-	-	10/13/13/13	-
3	EDO	B	607	-	-	0/1/1/1	-
2	MYR	B	603	-	-	8/13/13/13	-
2	MYR	A	602	-	-	4/13/13/13	-
4	GOR	B	608	-	-	0/6/14/14	0/4/4/4
3	EDO	A	608	-	-	1/1/1/1	-
3	EDO	A	607	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYR	B	606	-	-	6/13/13/13	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	610	GOR	C8-C4-C3	-2.64	116.88	118.69
4	B	608	GOR	C8-C4-C3	-2.59	116.92	118.69
4	A	611	GOR	C8-C4-C3	-2.57	116.93	118.69
2	B	605	MYR	C3-C2-C1	-2.44	108.14	114.51
4	B	609	GOR	C8-C4-C3	-2.29	117.12	118.69
2	A	604	MYR	C3-C2-C1	-2.15	108.91	114.51
2	B	606	MYR	C3-C2-C1	-2.11	109.00	114.51
2	B	603	MYR	O2-C1-C2	2.04	120.44	114.00

There are no chirality outliers.

All (89) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	B	601	MYR	C3-C4-C5-C6
2	B	603	MYR	C11-C10-C9-C8
4	B	609	GOR	C6-C5-C7-O2
4	B	609	GOR	C6-C5-C7-O3
4	B	609	GOR	C4-C5-C7-O2
4	B	609	GOR	C4-C5-C7-O3
2	A	602	MYR	C3-C4-C5-C6
2	A	605	MYR	C2-C3-C4-C5
2	A	604	MYR	C7-C8-C9-C10
2	B	601	MYR	C1-C2-C3-C4
2	B	604	MYR	C4-C5-C6-C7
2	B	602	MYR	C2-C3-C4-C5
2	B	606	MYR	C6-C7-C8-C9
2	B	605	MYR	C5-C6-C7-C8
2	B	604	MYR	C2-C3-C4-C5
2	A	604	MYR	C1-C2-C3-C4
2	A	605	MYR	C6-C7-C8-C9
2	A	601	MYR	C1-C2-C3-C4
2	A	601	MYR	C3-C4-C5-C6
2	A	603	MYR	C7-C8-C9-C10
2	B	602	MYR	C10-C11-C12-C13
2	A	602	MYR	C9-C10-C11-C12
2	A	605	MYR	C9-C10-C11-C12
2	A	601	MYR	C4-C5-C6-C7
2	A	602	MYR	C5-C6-C7-C8
2	A	604	MYR	C2-C3-C4-C5
2	B	605	MYR	C7-C8-C9-C10
2	A	605	MYR	C10-C11-C12-C13
4	A	611	GOR	C4-C5-C7-O2
4	A	611	GOR	C4-C5-C7-O3
2	A	603	MYR	C3-C4-C5-C6
2	B	606	MYR	C3-C4-C5-C6
2	B	604	MYR	C6-C7-C8-C9
4	A	611	GOR	C6-C5-C7-O2
4	A	611	GOR	C6-C5-C7-O3
2	A	605	MYR	C5-C6-C7-C8
2	A	603	MYR	C4-C5-C6-C7
4	B	609	GOR	C9-C8-N-O4
2	B	603	MYR	C3-C4-C5-C6
4	A	610	GOR	C4-C8-N-O4
2	A	603	MYR	C1-C2-C3-C4
2	B	602	MYR	C11-C12-C13-C14

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

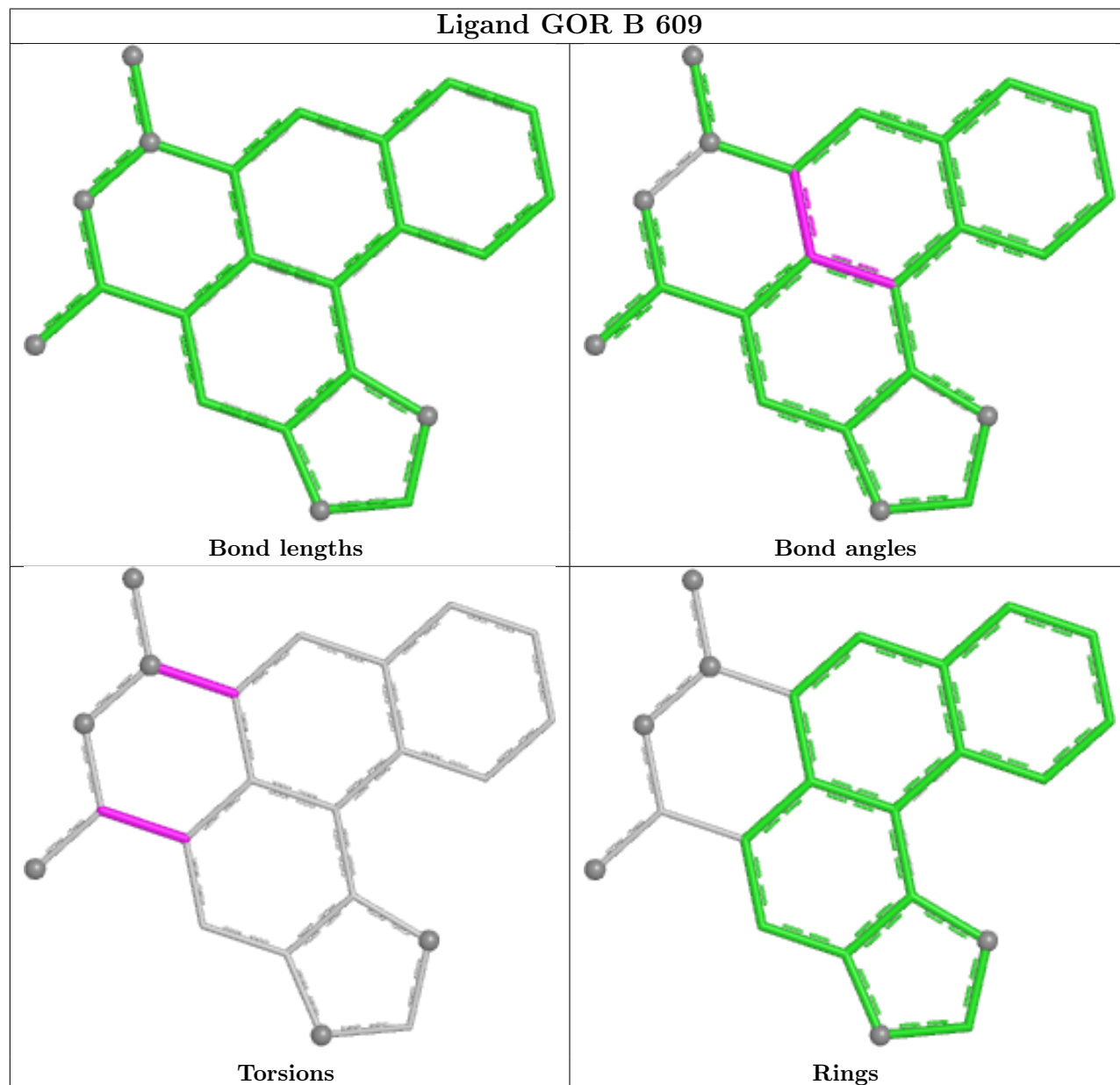
There are no ring outliers.

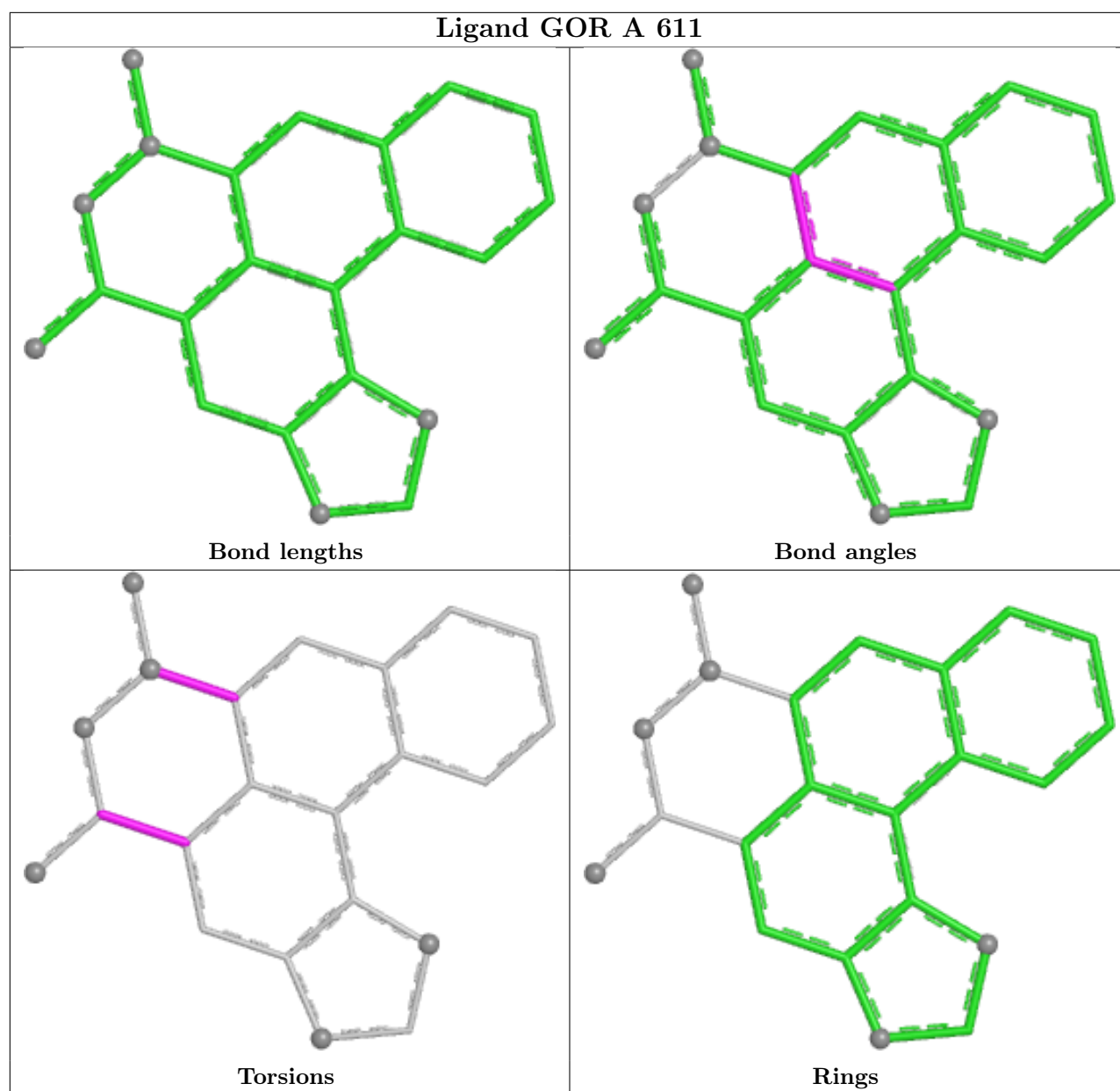
9 monomers are involved in 14 short contacts:

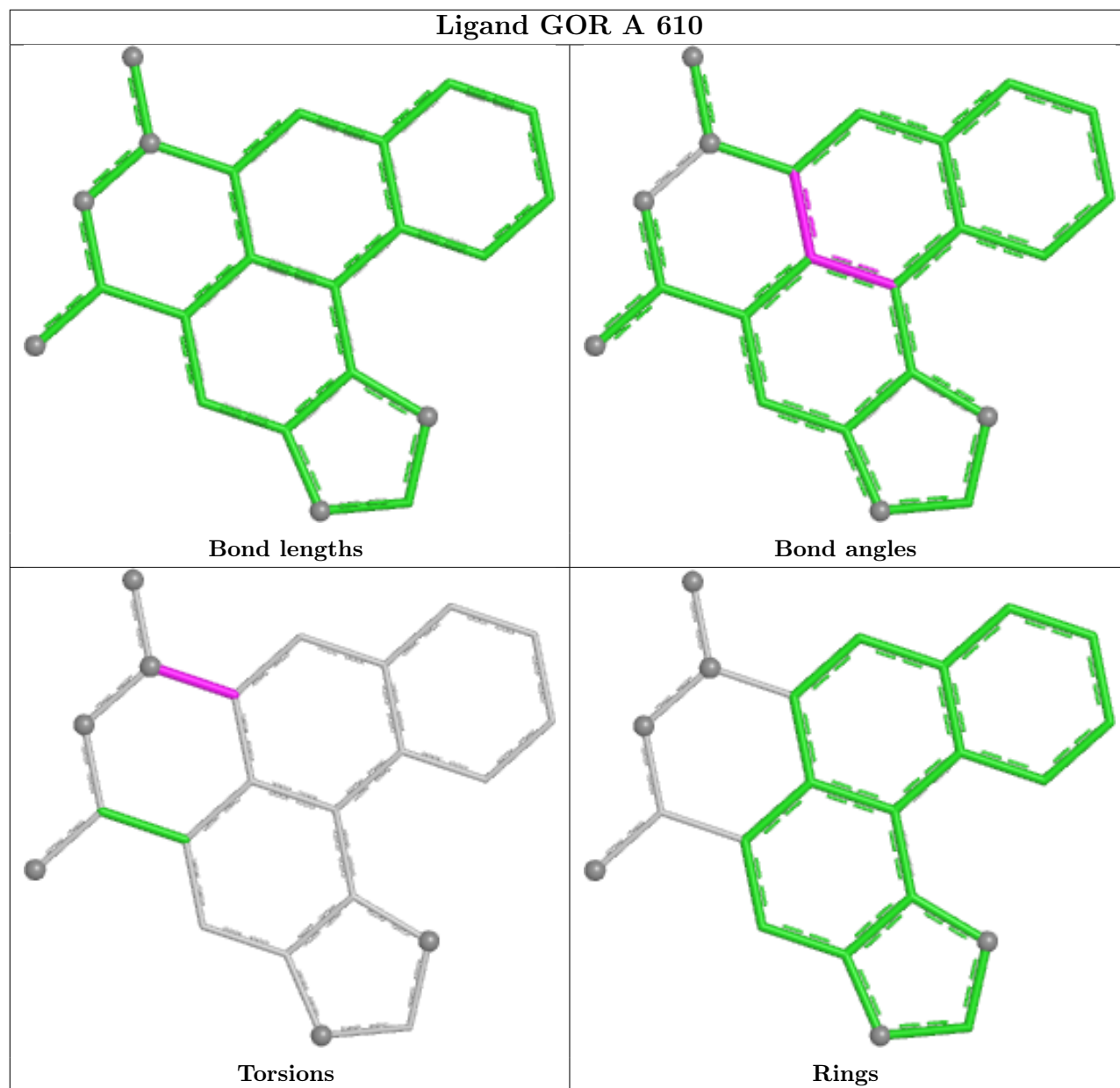
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	609	GOR	2	0
2	A	601	MYR	4	0
2	B	601	MYR	1	0
4	A	611	GOR	1	0
4	A	610	GOR	1	0
2	B	604	MYR	2	0
2	A	602	MYR	1	0
4	B	608	GOR	1	0
2	B	606	MYR	1	0

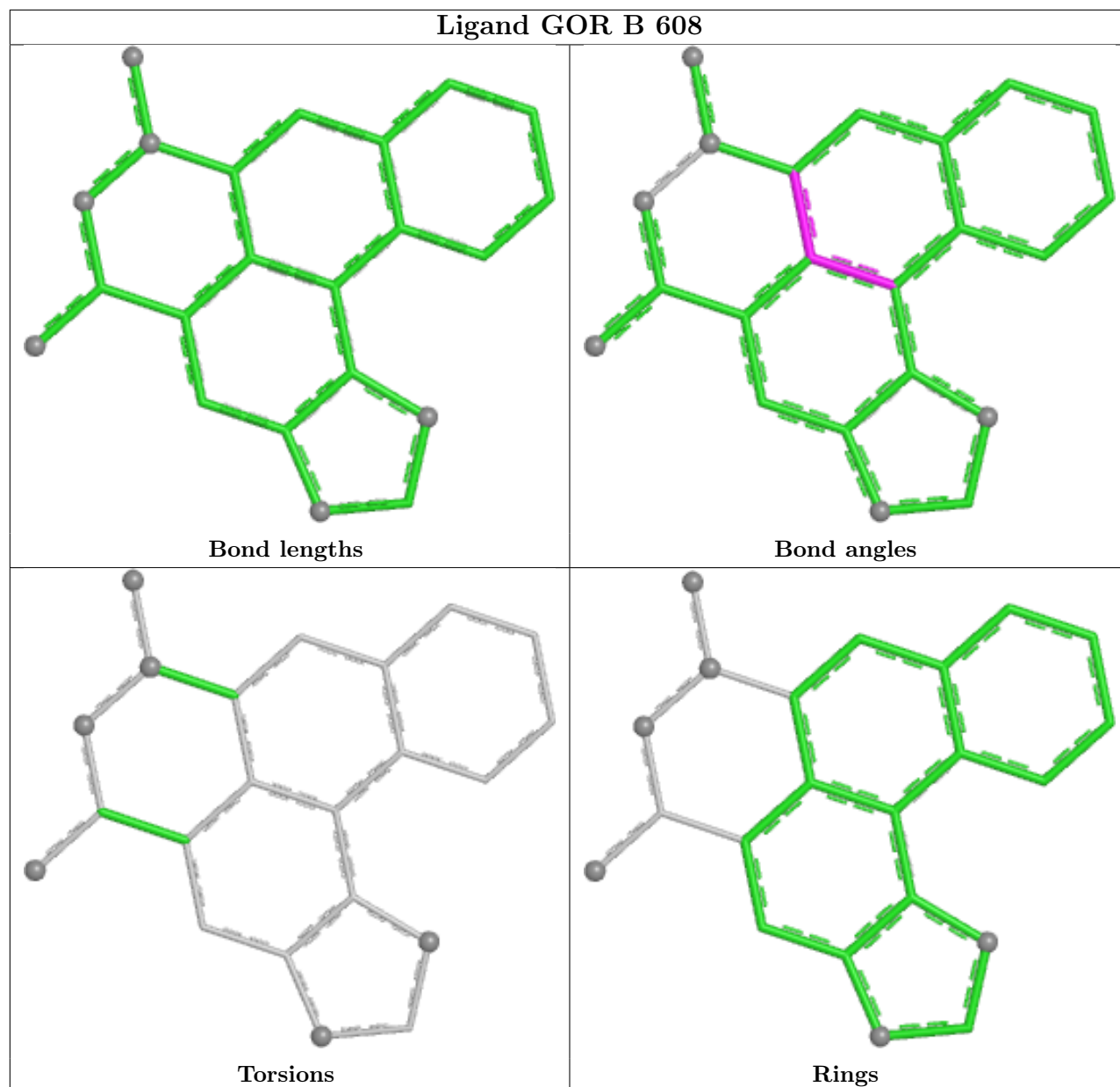
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	582/609 (95%)	0.66	35 (6%)	27 29	22, 46, 69, 96	3 (0%)
1	B	582/609 (95%)	0.74	57 (9%)	13 13	20, 46, 72, 94	1 (0%)
All	All	1164/1218 (95%)	0.70	92 (7%)	18 20	20, 46, 72, 96	4 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	584	GLY	5.0
1	A	584	GLY	4.3
1	A	509	PHE	4.1
1	B	555	VAL	3.7
1	B	470	SER	3.6
1	B	452	TYR	3.6
1	B	533	VAL	3.6
1	B	464	HIS	3.6
1	B	481	LEU	3.5
1	A	555	VAL	3.4
1	A	561	ALA	3.3
1	B	516	LEU	3.3
1	B	467	THR	3.1
1	B	468	PRO	3.0
1	A	564	LYS	3.0
1	A	513	ILE	3.0
1	B	583	LEU	3.0
1	B	497	TYR	2.9
1	B	469	VAL	2.8
1	A	481	LEU	2.8
1	A	583	LEU	2.8
1	B	463	LEU	2.8
1	B	507	PHE	2.7
1	B	558	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	415	VAL	2.7
1	A	443	ALA	2.7
1	A	551	PHE	2.7
1	B	513	ILE	2.7
1	B	218[A]	ARG	2.7
1	A	568	PHE	2.6
1	B	565	GLU	2.6
1	B	551	PHE	2.6
1	B	475	LYS	2.5
1	B	546	ALA	2.5
1	A	480	SER	2.5
1	A	502	PHE	2.4
1	B	582	ALA	2.4
1	A	462	VAL	2.4
1	B	473	VAL	2.4
1	A	559	CYS	2.4
1	B	283	LEU	2.4
1	B	509	PHE	2.4
1	A	439	LYS	2.4
1	B	474	THR	2.4
1	B	498	VAL	2.4
1	A	207	GLY	2.3
1	B	108	ASP	2.3
1	B	396	GLU	2.3
1	A	408	LEU	2.3
1	B	502	PHE	2.3
1	B	539	ALA	2.3
1	B	493	VAL	2.3
1	A	507	PHE	2.3
1	B	305	LEU	2.2
1	B	552	ALA	2.2
1	A	533	VAL	2.2
1	A	204	GLN	2.2
1	A	511	ALA	2.2
1	A	546	ALA	2.2
1	B	504	ALA	2.2
1	B	569	ALA	2.2
1	A	452	TYR	2.2
1	A	544	LEU	2.2
1	A	504	ALA	2.2
1	B	500	LYS	2.2
1	B	554	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	416	PRO	2.1
1	B	544	LEU	2.1
1	B	204	GLN	2.1
1	A	467	THR	2.1
1	B	560	LYS	2.1
1	B	529	LEU	2.1
1	B	490	ALA	2.1
1	B	581	ALA	2.1
1	A	79	THR	2.1
1	A	455	VAL	2.1
1	B	532	LEU	2.1
1	B	92	ALA	2.1
1	A	563	ASP	2.1
1	B	13	ASP	2.1
1	A	156	PHE	2.0
1	B	465	GLU	2.0
1	B	517	SER	2.0
1	B	478	THR	2.0
1	B	540	THR	2.0
1	B	440	HIS	2.0
1	B	418	VAL	2.0
1	A	575	LEU	2.0
1	B	559	CYS	2.0
1	A	218[A]	ARG	2.0
1	A	565	GLU	2.0
1	B	557	LYS	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](#)

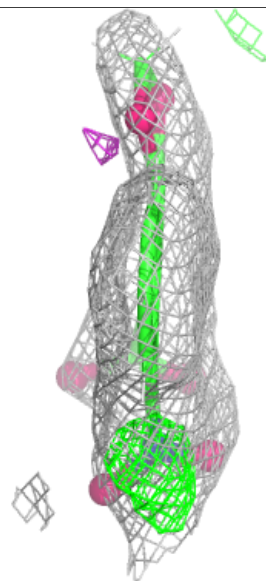
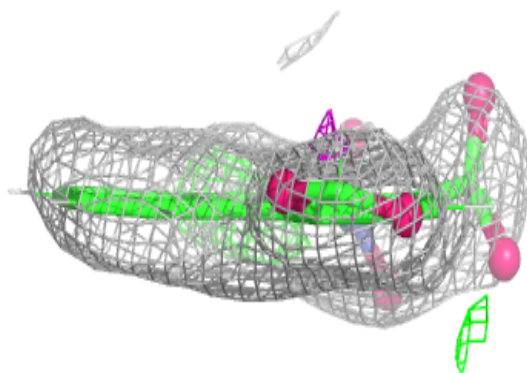
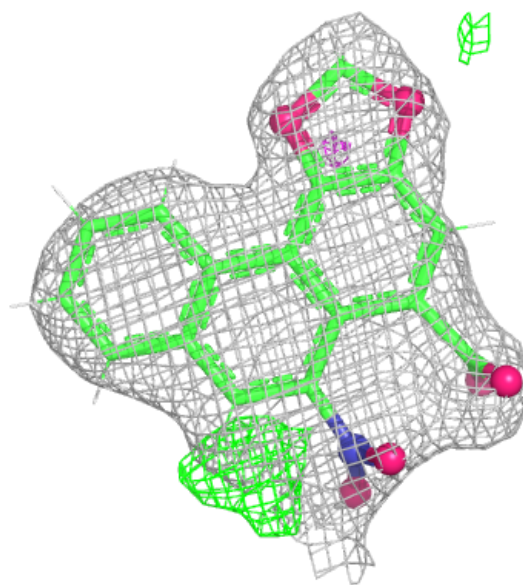
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MYR	B	601	16/16	0.79	0.21	26,49,67,67	43
3	EDO	A	607	4/4	0.81	0.15	44,62,74,74	0
2	MYR	A	601	16/16	0.82	0.20	34,46,62,65	43
4	GOR	B	609	23/23	0.82	0.16	32,48,59,67	31
2	MYR	B	604	16/16	0.83	0.23	37,55,70,71	43
4	GOR	A	611	23/23	0.83	0.14	34,44,64,69	31
2	MYR	B	605	16/16	0.83	0.17	45,59,70,74	0
3	EDO	A	608	4/4	0.84	0.12	42,63,72,78	0
2	MYR	A	606	16/16	0.85	0.19	31,44,59,61	43
2	MYR	A	605	16/16	0.86	0.16	40,54,70,74	0
2	MYR	B	602	16/16	0.86	0.17	31,48,61,65	43
2	MYR	A	604	16/16	0.88	0.16	39,56,62,71	43
3	EDO	A	609	4/4	0.89	0.11	42,51,52,52	0
4	GOR	A	610	23/23	0.89	0.10	31,37,47,53	0
2	MYR	A	602	16/16	0.89	0.14	32,52,67,68	0
4	GOR	B	608	23/23	0.89	0.10	27,37,45,55	0
2	MYR	B	606	16/16	0.89	0.18	27,43,66,71	43
2	MYR	A	603	16/16	0.90	0.14	28,51,68,70	0
2	MYR	B	603	16/16	0.90	0.13	34,46,63,72	0
3	EDO	B	607	4/4	0.91	0.12	44,53,57,58	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.

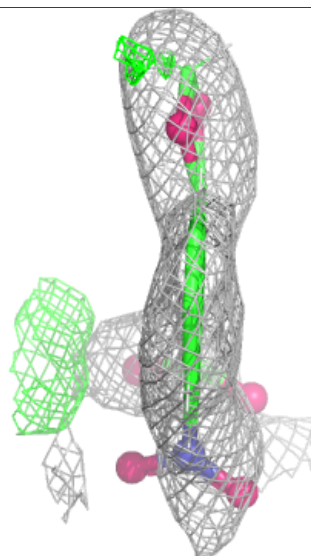
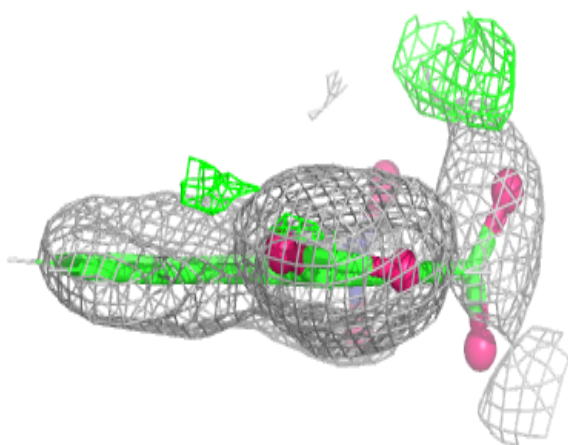
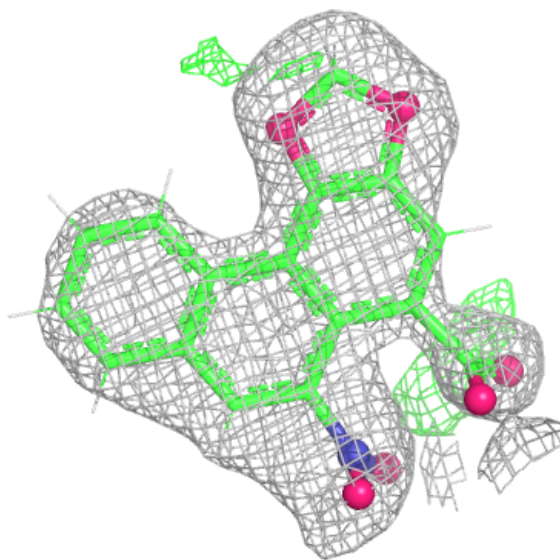
Electron density around GOR B 609:

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



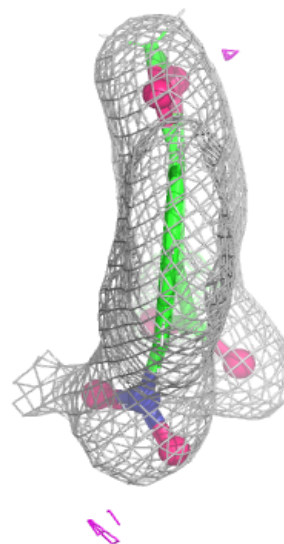
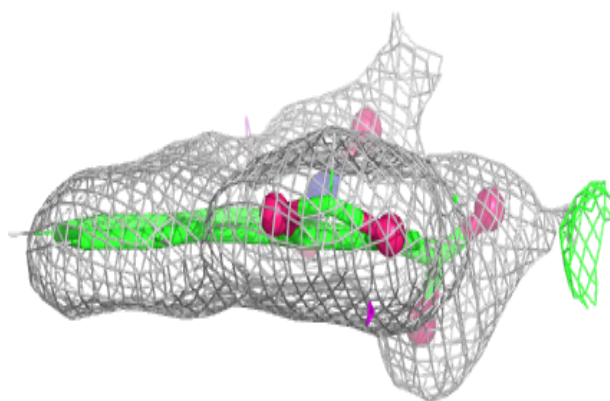
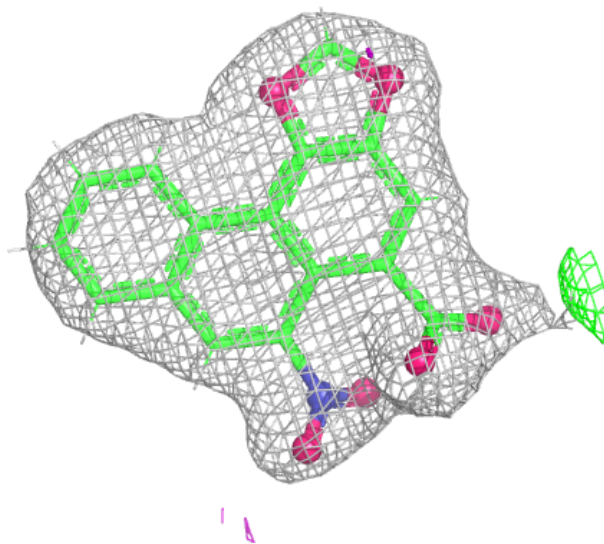
Electron density around GOR A 611:

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



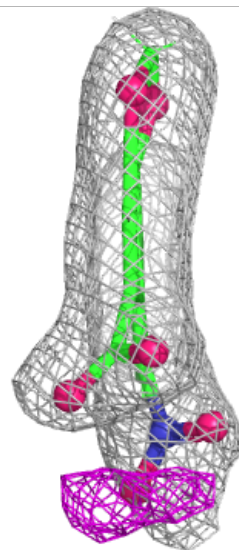
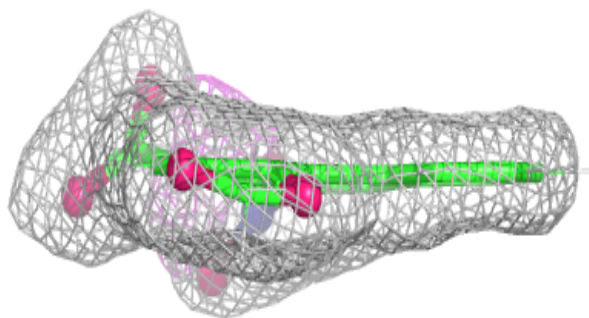
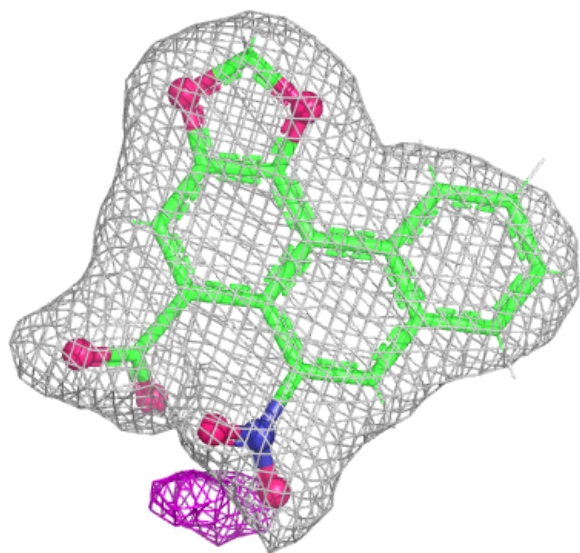
Electron density around GOR A 610:

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



Electron density around GOR B 608:

$2mF_o-DF_c$ (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.