



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:49 AM UTC

PDB ID : 8RCP / pdb_00008rcp
Title : Structure of Human Serum Albumin in complex with Myristic Acid
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

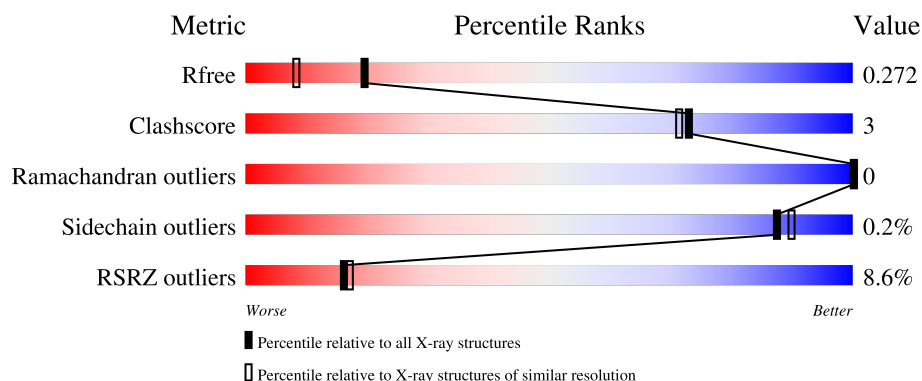
1 Overall quality at a glance

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	7% 89% 7% .
1	B	609	9% 88% 7% .

2 Entry composition [i](#)

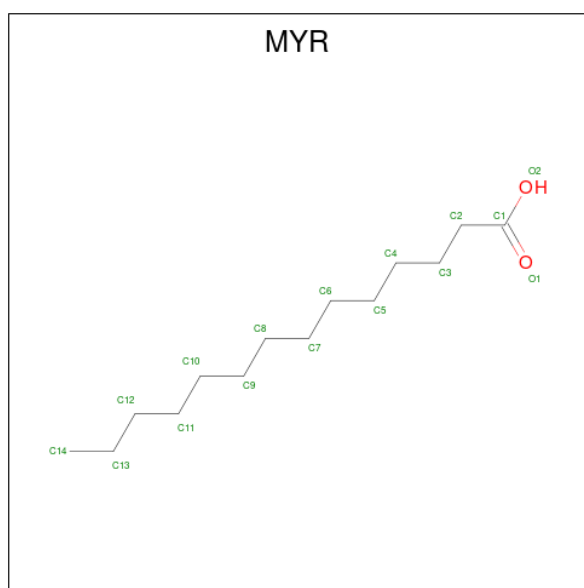
There are 4 unique types of molecules in this entry. The entry contains 19495 atoms, of which 9397 are hydrogens and 0 are deuteriums.

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
			9100	2906	4502	782	869	41			
1	B	582	Total	C	H	N	O	S	0	4	0
			9012	2890	4435	776	870	41			

- Molecule 2 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$) (labeled as "Ligand of Interest" by depositor).



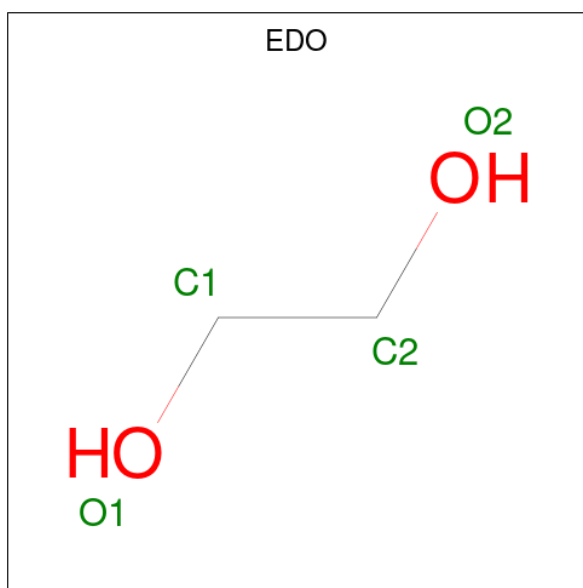
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			44	14	28	2		
2	A	1	Total	C	H	O	0	0
			44	14	28	2		
2	A	1	Total	C	H	O	0	0
			44	14	28	2		
2	A	1	Total	C	H	O	0	0
			44	14	28	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			44	14	28	2		
2	A	1	Total	C	H	O	0	0
			44	14	28	2		
2	A	1	Total	C	H	O	0	0
			44	14	28	2		
2	A	1	Total	C	H	O	0	0
			44	14	28	2		
2	B	1	Total	C	H	O	0	0
			44	14	28	2		
2	B	1	Total	C	H	O	0	0
			44	14	28	2		
2	B	1	Total	C	H	O	0	0
			44	14	28	2		
2	B	1	Total	C	H	O	0	0
			44	14	28	2		
2	B	1	Total	C	H	O	0	0
			44	14	28	2		
2	B	1	Total	C	H	O	0	0
			44	14	28	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

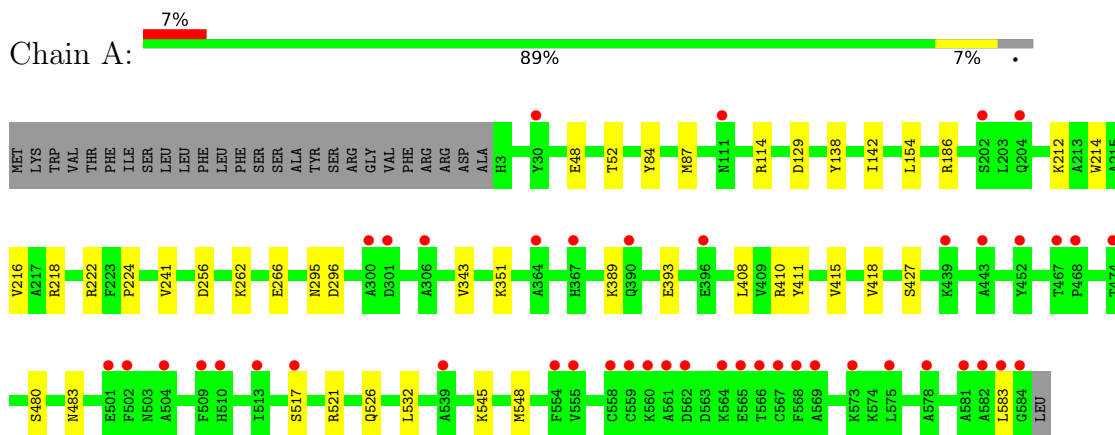
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	327	Total	O	0	0
			327	327		
4	B	332	Total	O	0	0
			332	332		

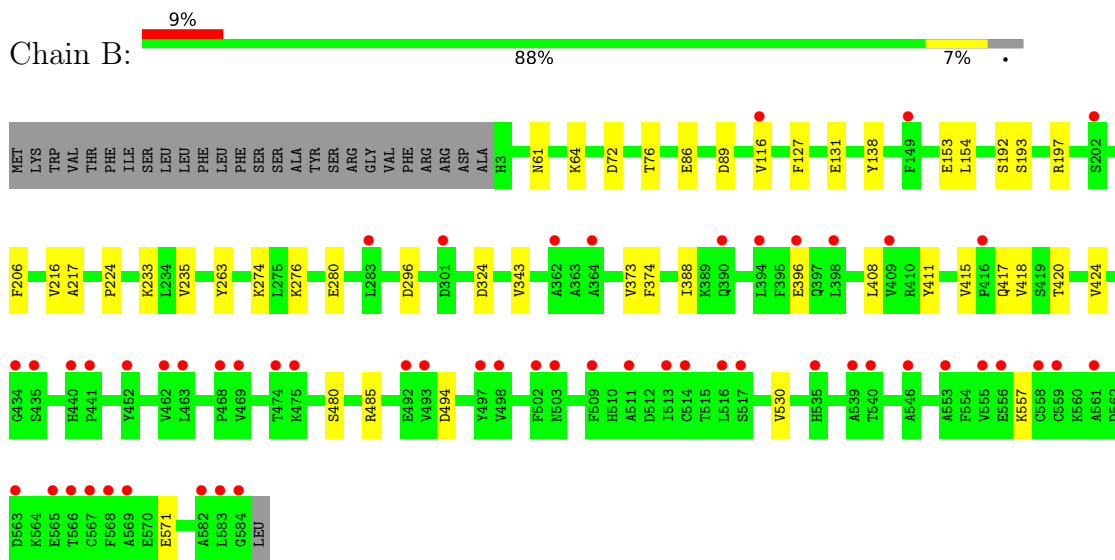
3 Residue-property plots [i](#)

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	95.73Å 38.56Å 183.56Å 90.00° 104.66° 90.00°	Depositor
Resolution (Å)	74.15 – 1.90 74.15 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (74.15-1.90) 98.7 (74.15-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.224 , 0.269 0.225 , 0.272	Depositor DCC
R_{free} test set	5045 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19495	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 48.96 % 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 7.9912e-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: 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	0.46	0/4699	0.57	0/6344
1	B	0.45	0/4680	0.57	0/6328
All	All	0.46	0/9379	0.57	0/12672

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	4598	4502	4490	27	1
1	B	4577	4435	4425	31	0
2	A	128	224	216	4	0
2	B	128	224	216	8	0
3	A	4	6	6	0	0
3	B	4	6	6	0	0
4	A	327	0	0	1	0
4	B	332	0	0	4	0
All	All	10098	9397	9359	61	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (61) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:GLN:NE2	1:B:494:ASP:OD2	2.25	0.69
1:A:84:TYR:HB3	1:A:87:MET:HE3	1.76	0.68
1:B:408:LEU:HD22	1:B:530:VAL:CG2	2.30	0.61
1:A:415:VAL:HG12	1:A:418:VAL:HG23	1.83	0.59
1:B:138:TYR:HB3	2:B:601:MYR:H92	1.84	0.59
1:B:388:ILE:HG13	2:B:603:MYR:H82	1.85	0.58
1:B:415:VAL:HG12	1:B:415:VAL:O	2.05	0.57
1:B:415:VAL:HG12	1:B:418:VAL:HG23	1.84	0.57
1:B:324:ASP:OD1	4:B:701:HOH:O	2.18	0.56
2:B:603:MYR:H91	2:B:603:MYR:H132	1.87	0.56
1:A:262:LYS:HE3	1:A:266:GLU:OE2	2.07	0.55
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.72	0.55
1:A:545:LYS:HA	1:A:548:MET:HE3	1.89	0.54
1:A:389:LYS:O	1:A:393:GLU:HG3	2.08	0.54
1:A:241:VAL:HG22	1:A:256:ASP:HB3	1.91	0.53
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.44	0.53
1:B:420:THR:O	1:B:424:VAL:HG23	2.09	0.53
1:B:154:LEU:HD12	2:B:608:MYR:H101	1.92	0.52
1:A:410:ARG:HD2	1:A:411:TYR:CE1	2.44	0.52
1:A:548:MET:HG2	2:A:605:MYR:H42	1.91	0.51
1:A:548:MET:HG2	2:A:605:MYR:H22	1.93	0.51
1:B:61:ASN:OD1	1:B:64:LYS:HE2	2.13	0.49
1:B:86:GLU:O	1:B:89:ASP:HB2	2.13	0.48
1:B:233:LYS:HE2	1:B:263:TYR:CE1	2.49	0.48
1:B:274:LYS:HE3	1:B:296:ASP:HA	1.96	0.47
1:B:557:LYS:NZ	1:B:571:GLU:OE1	2.44	0.47
1:B:216:VAL:HG22	1:B:235:VAL:HG21	1.95	0.47
1:B:197:ARG:NH2	4:B:715:HOH:O	2.47	0.46
1:A:410:ARG:HH11	1:A:410:ARG:HG3	1.81	0.46
1:A:222:ARG:HD3	1:A:295:ASN:OD1	2.15	0.46
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.98	0.46
1:B:116:VAL:O	4:B:702:HOH:O	2.20	0.45
1:A:48:GLU:O	1:A:52:THR:HG23	2.16	0.45
1:A:532:LEU:HD11	1:A:583:LEU:HD11	1.97	0.45
1:A:480[B]:SER:OG	1:A:483:ASN:OD1	2.35	0.45
1:B:72:ASP:O	1:B:76:THR:HG23	2.17	0.45
1:A:408:LEU:HD21	1:A:526:GLN:HB3	1.98	0.45
2:B:601:MYR:H141	2:B:608:MYR:H92	1.99	0.44
1:A:138:TYR:O	1:A:142:ILE:HG12	2.17	0.44
1:B:411:TYR:HB3	2:B:604:MYR:H132	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LYS:HD2	2:A:606:MYR:H32	2.00	0.44
1:A:389:LYS:HG3	4:A:720:HOH:O	2.18	0.43
1:A:186:ARG:HA	2:A:608:MYR:H71	1.99	0.43
1:A:521:ARG:HH11	1:A:521:ARG:HG3	1.83	0.43
1:B:396:GLU:HA	4:B:929:HOH:O	2.19	0.43
1:A:408:LEU:HD13	1:A:427:SER:CB	2.48	0.43
1:A:408:LEU:HD13	1:A:427:SER:HB2	2.01	0.42
1:A:415:VAL:CG1	1:A:418:VAL:HG23	2.47	0.42
2:B:603:MYR:H132	2:B:604:MYR:H42	2.01	0.42
1:B:206:PHE:CZ	1:B:480:SER:HA	2.54	0.42
1:B:127:PHE:CE1	1:B:131:GLU:HG3	2.55	0.42
1:B:224:PRO:HD2	1:B:296:ASP:HB3	2.02	0.42
1:B:153:GLU:OE2	1:B:192:SER:OG	2.37	0.42
1:B:233:LYS:HE2	1:B:263:TYR:CZ	2.55	0.42
1:B:388:ILE:CG1	2:B:603:MYR:H82	2.49	0.41
1:B:193:SER:O	1:B:197:ARG:HG3	2.20	0.41
1:B:217:ALA:HB3	1:B:343:VAL:HG13	2.02	0.41
1:A:154:LEU:HD12	1:A:154:LEU:HA	1.88	0.41
1:A:212:LYS:O	1:A:216:VAL:HG23	2.21	0.40
1:B:485:ARG:HD2	1:B:485:ARG:C	2.46	0.40
1:B:276:LYS:NZ	1:B:280:GLU:OE2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:HH22	1:A:129:ASP:OD1[2_546]	1.59	0.01

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%)	573 (98%)	10 (2%)	0	100	100
1	B	584/609 (96%)	575 (98%)	9 (2%)	0	100	100
All	All	1167/1218 (96%)	1148 (98%)	19 (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	500/533 (94%)	497 (99%)	3 (1%)	78	81
1	B	494/533 (93%)	494 (100%)	0	100	100
All	All	994/1066 (93%)	991 (100%)	3 (0%)	87	88

All (3) 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	517	SER

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	288	HIS
1	A	367	HIS
1	A	580	GLN
1	B	3	HIS
1	B	99	ASN
1	B	580	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	B	609	-	3,3,3	0.61	0	2,2,2	0.20	0
2	MYR	A	607	-	15,15,15	0.18	0	15,15,15	0.30	0
2	MYR	A	605	-	15,15,15	0.14	0	15,15,15	0.34	0
2	MYR	B	601	-	15,15,15	0.20	0	15,15,15	0.40	0
2	MYR	B	604	-	15,15,15	0.27	0	15,15,15	0.33	0
2	MYR	A	604	-	15,15,15	0.23	0	15,15,15	0.36	0
2	MYR	A	601	-	15,15,15	0.16	0	15,15,15	0.26	0
2	MYR	A	606	-	15,15,15	0.29	0	15,15,15	0.50	0
2	MYR	B	602	-	15,15,15	0.28	0	15,15,15	0.43	0
2	MYR	B	606	-	15,15,15	0.26	0	15,15,15	0.34	0
2	MYR	A	608	-	15,15,15	0.18	0	15,15,15	0.29	0
2	MYR	B	608	-	15,15,15	0.16	0	15,15,15	0.38	0
3	EDO	A	609	-	3,3,3	0.50	0	2,2,2	0.09	0
2	MYR	B	607	-	15,15,15	0.26	0	15,15,15	0.20	0
2	MYR	B	603	-	15,15,15	0.26	0	15,15,15	0.50	0
2	MYR	B	605	-	15,15,15	0.13	0	15,15,15	0.19	0
2	MYR	A	603	-	15,15,15	0.42	0	15,15,15	0.33	0
2	MYR	A	602	-	15,15,15	0.22	0	15,15,15	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	609	-	-	0/1/1/1	-
2	MYR	A	607	-	-	7/13/13/13	-
2	MYR	A	605	-	-	4/13/13/13	-
2	MYR	B	601	-	-	3/13/13/13	-
2	MYR	B	604	-	-	3/13/13/13	-
2	MYR	A	604	-	-	4/13/13/13	-
2	MYR	A	601	-	-	8/13/13/13	-
2	MYR	A	606	-	-	6/13/13/13	-
2	MYR	B	602	-	-	3/13/13/13	-
2	MYR	B	606	-	-	5/13/13/13	-
2	MYR	A	608	-	-	7/13/13/13	-
2	MYR	B	608	-	-	4/13/13/13	-
3	EDO	A	609	-	-	0/1/1/1	-
2	MYR	B	607	-	-	5/13/13/13	-
2	MYR	B	603	-	-	8/13/13/13	-
2	MYR	B	605	-	-	6/13/13/13	-
2	MYR	A	603	-	-	7/13/13/13	-
2	MYR	A	602	-	-	6/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	606	MYR	C1-C2-C3-C4
2	A	601	MYR	C1-C2-C3-C4
2	A	606	MYR	C1-C2-C3-C4
2	B	603	MYR	C1-C2-C3-C4
2	A	601	MYR	C6-C7-C8-C9
2	B	607	MYR	C10-C11-C12-C13
2	A	601	MYR	C10-C11-C12-C13
2	A	607	MYR	C1-C2-C3-C4
2	A	606	MYR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	B	608	MYR	C7-C8-C9-C10
2	A	606	MYR	C2-C3-C4-C5
2	A	602	MYR	C6-C7-C8-C9
2	A	603	MYR	C2-C3-C4-C5
2	B	607	MYR	C2-C3-C4-C5
2	A	608	MYR	C11-C12-C13-C14
2	B	601	MYR	C1-C2-C3-C4
2	A	608	MYR	C10-C11-C12-C13
2	A	601	MYR	C11-C10-C9-C8
2	B	604	MYR	C2-C3-C4-C5
2	A	608	MYR	C11-C10-C9-C8
2	A	608	MYR	C3-C4-C5-C6
2	A	601	MYR	C7-C8-C9-C10
2	A	605	MYR	C1-C2-C3-C4
2	A	608	MYR	C2-C3-C4-C5
2	B	603	MYR	C2-C3-C4-C5
2	A	608	MYR	C1-C2-C3-C4
2	A	602	MYR	C11-C12-C13-C14
2	B	603	MYR	C4-C5-C6-C7
2	A	607	MYR	C11-C10-C9-C8
2	B	605	MYR	C3-C4-C5-C6
2	B	607	MYR	C9-C10-C11-C12
2	B	603	MYR	C3-C4-C5-C6
2	B	605	MYR	C2-C3-C4-C5
2	B	608	MYR	C1-C2-C3-C4
2	A	603	MYR	C1-C2-C3-C4
2	A	602	MYR	C4-C5-C6-C7
2	A	607	MYR	C10-C11-C12-C13
2	A	607	MYR	C2-C3-C4-C5
2	B	606	MYR	C2-C3-C4-C5
2	A	603	MYR	C3-C4-C5-C6
2	A	605	MYR	C9-C10-C11-C12
2	B	608	MYR	C6-C7-C8-C9
2	B	601	MYR	C11-C10-C9-C8
2	B	608	MYR	C9-C10-C11-C12
2	A	603	MYR	C5-C6-C7-C8
2	A	602	MYR	C3-C4-C5-C6
2	B	606	MYR	C4-C5-C6-C7
2	A	601	MYR	C3-C4-C5-C6
2	B	602	MYR	C3-C4-C5-C6
2	A	603	MYR	C10-C11-C12-C13
2	A	604	MYR	O2-C1-C2-C3

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

There are no ring outliers.

7 monomers are involved in 12 short contacts:

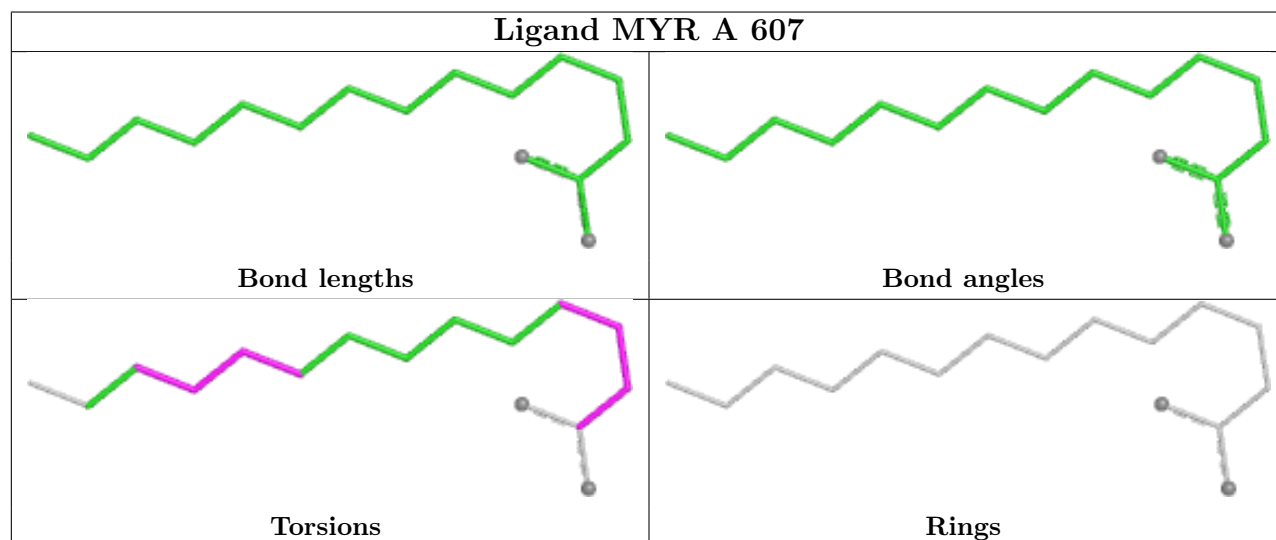
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	605	MYR	2	0
2	B	601	MYR	2	0

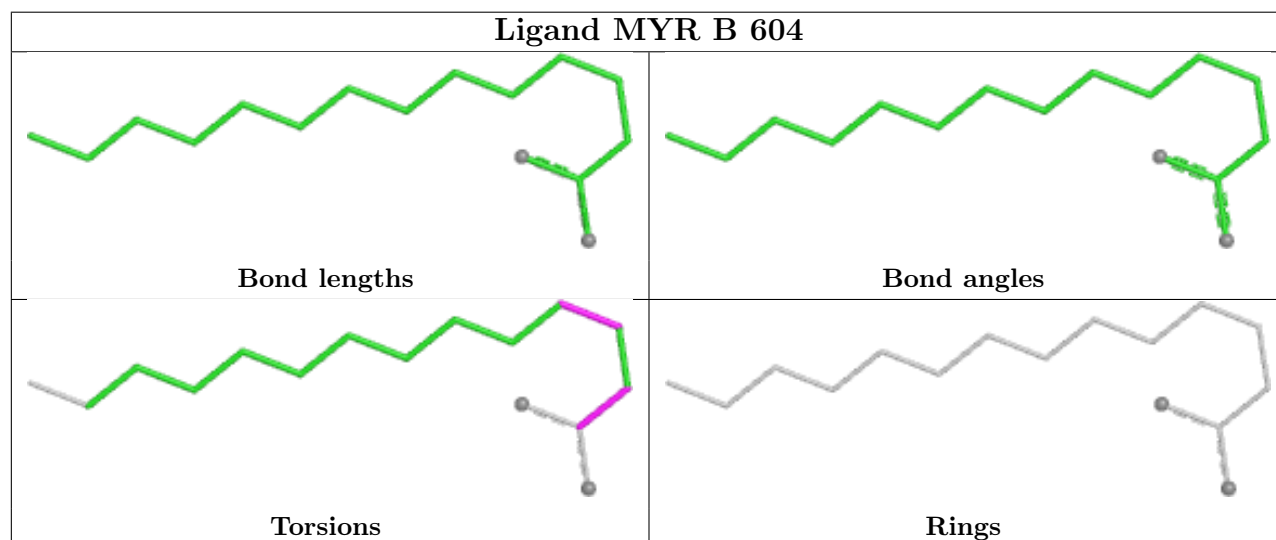
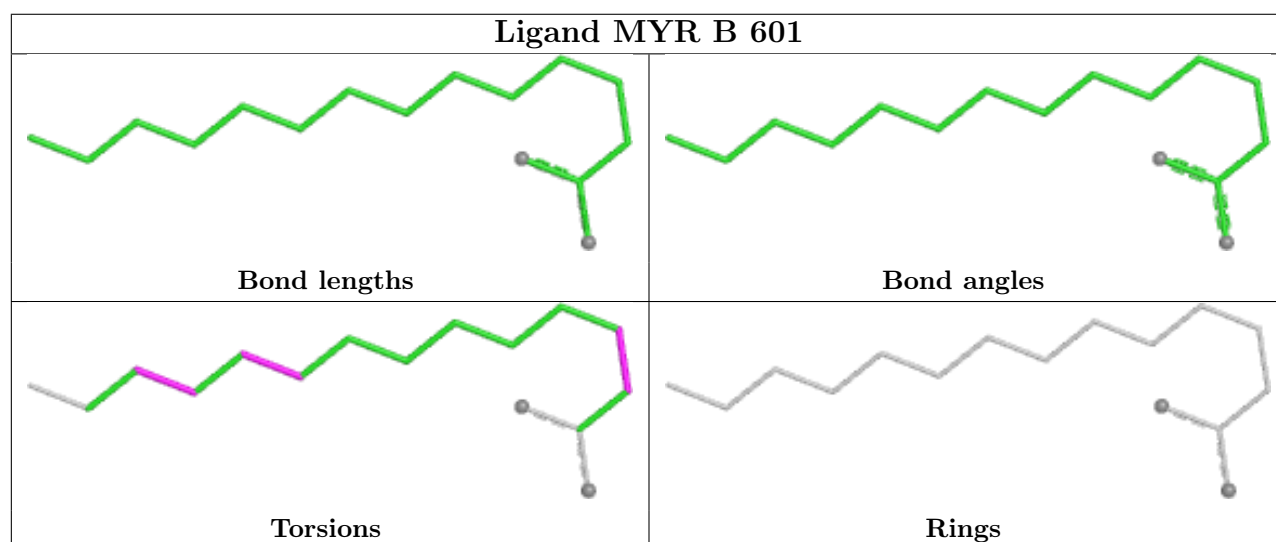
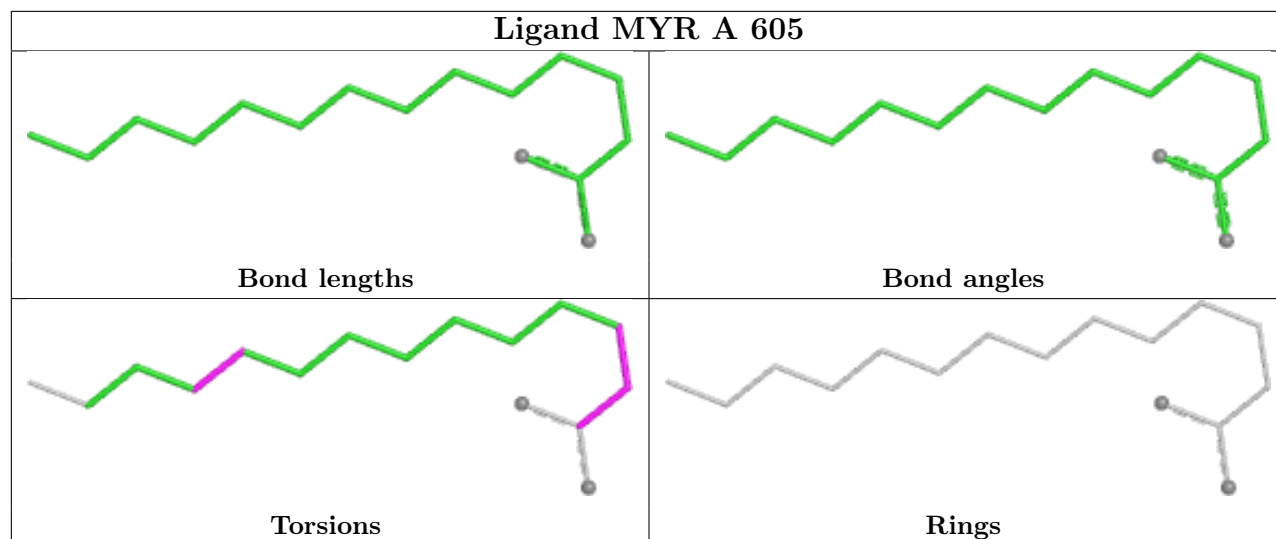
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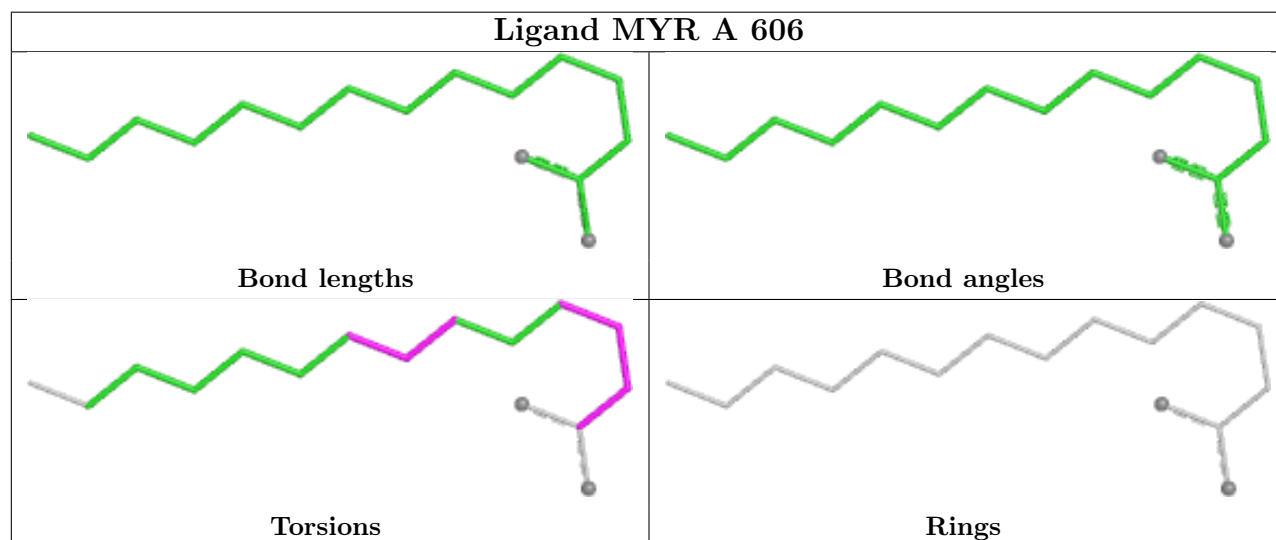
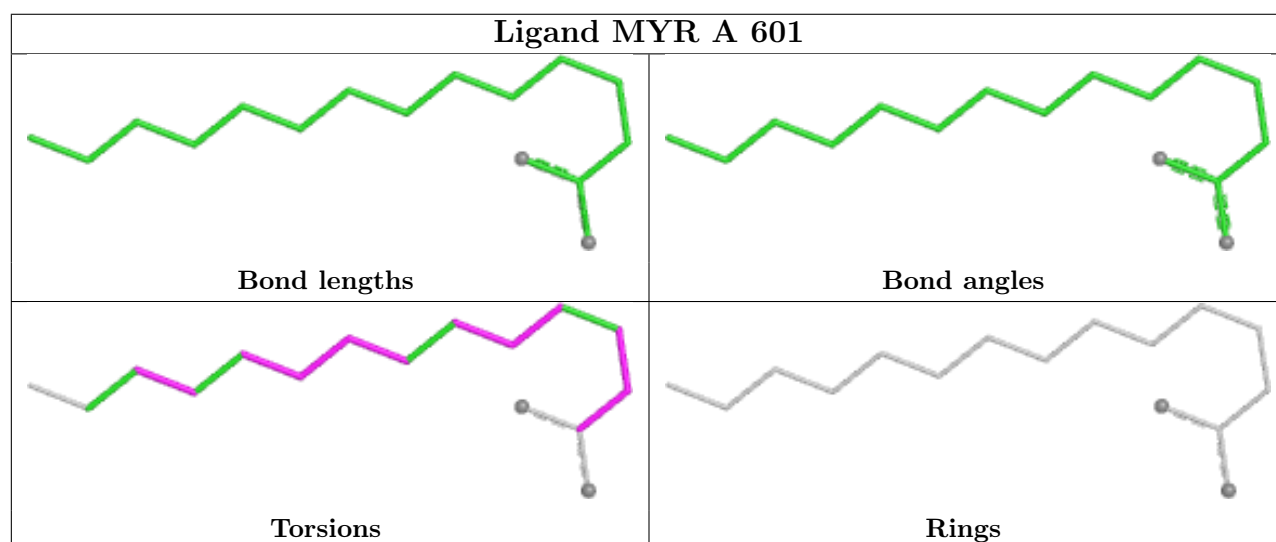
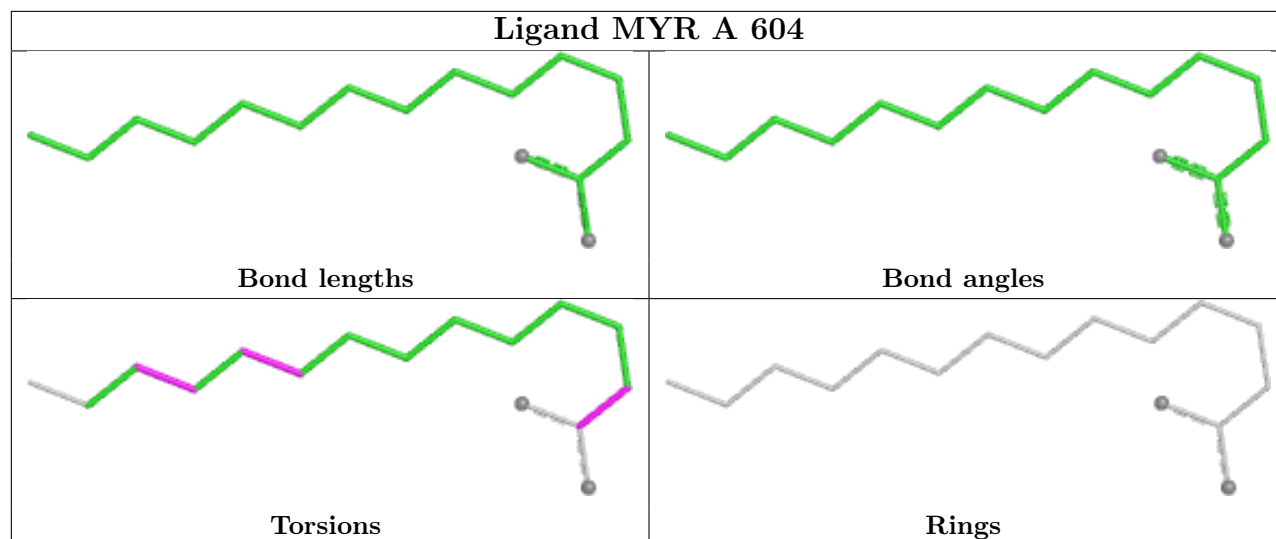
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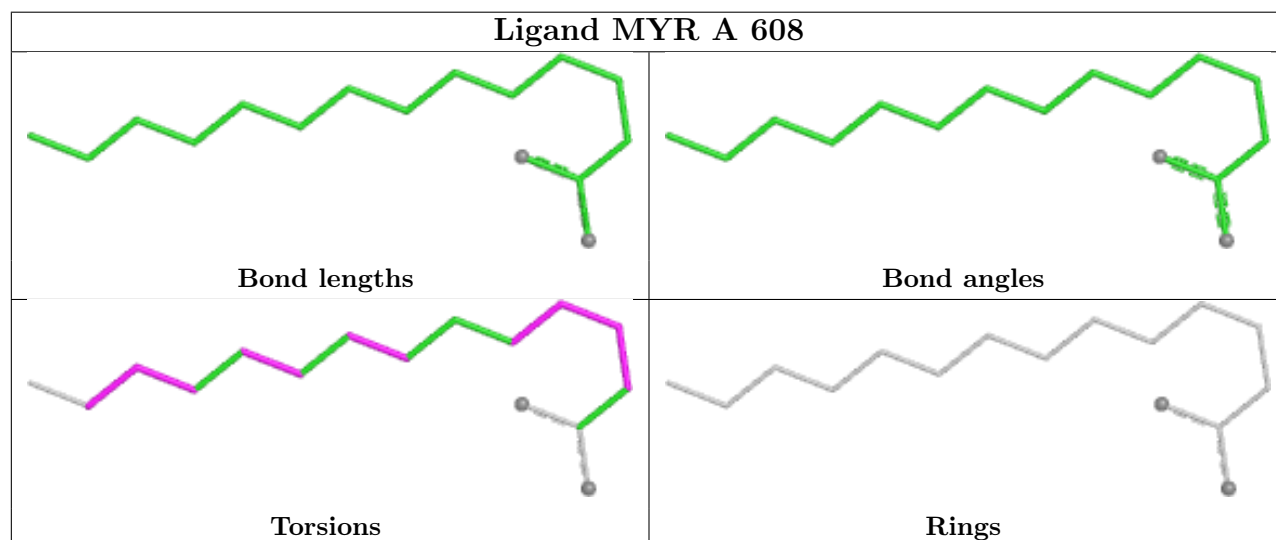
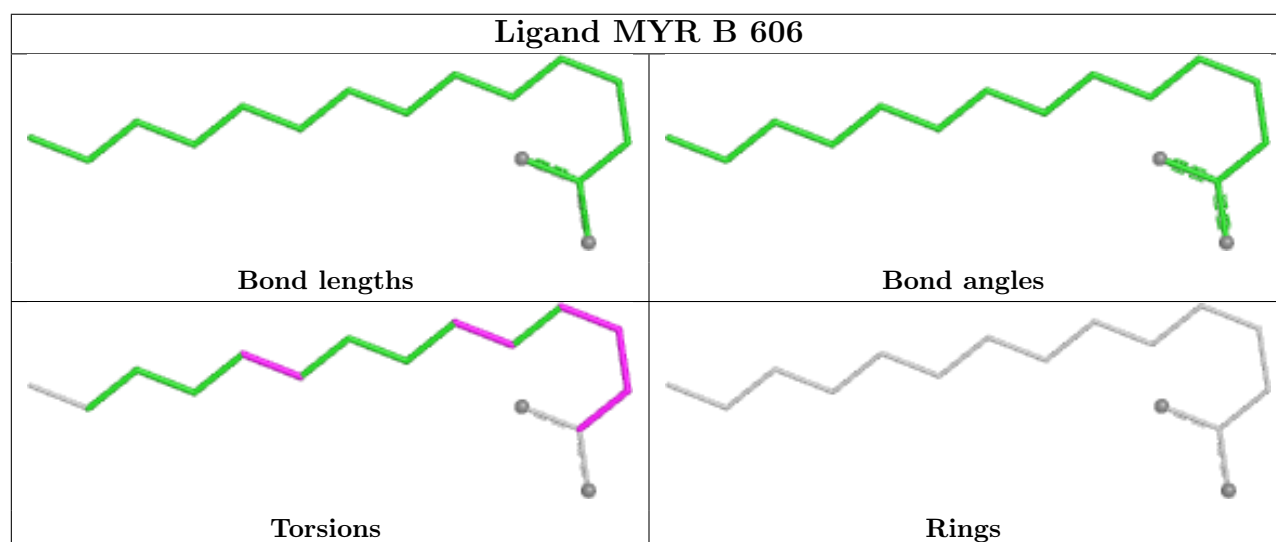
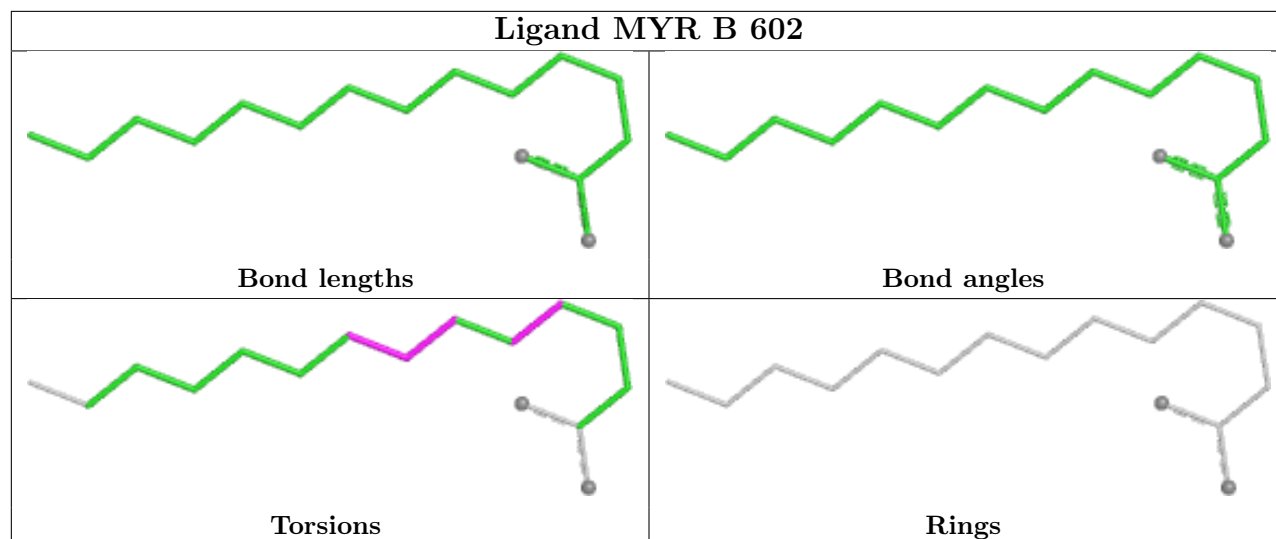
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	604	MYR	2	0
2	A	606	MYR	1	0
2	A	608	MYR	1	0
2	B	608	MYR	2	0
2	B	603	MYR	4	0

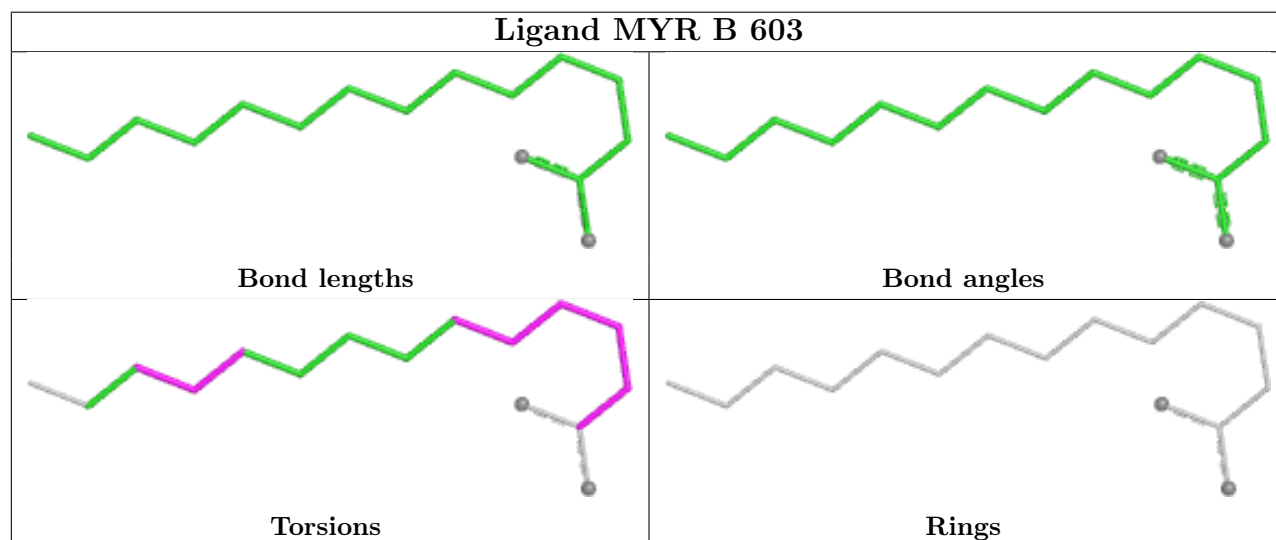
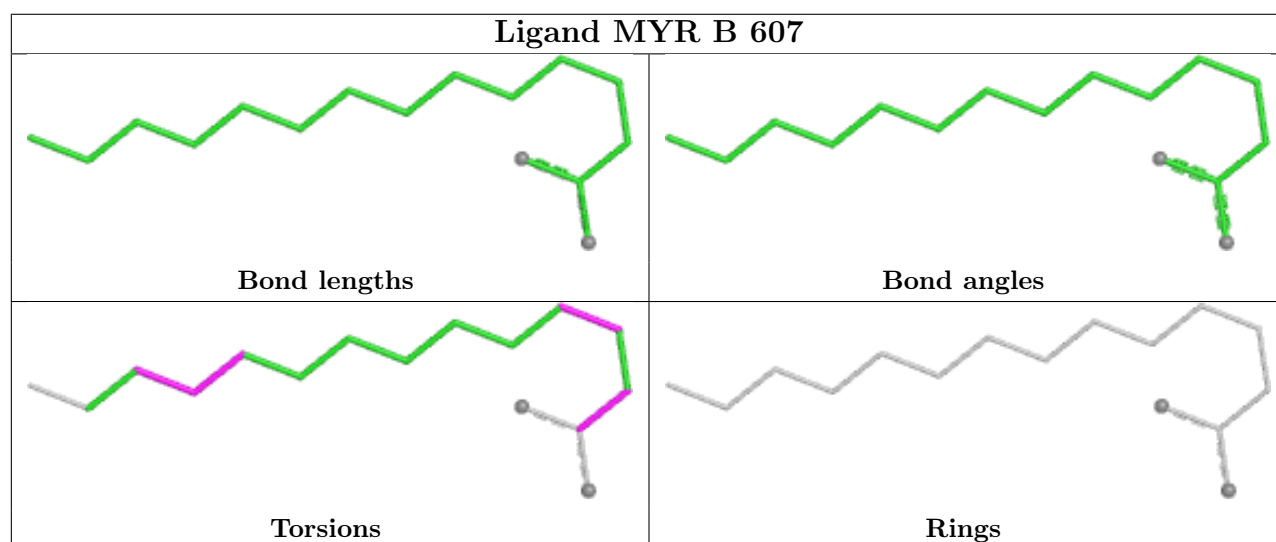
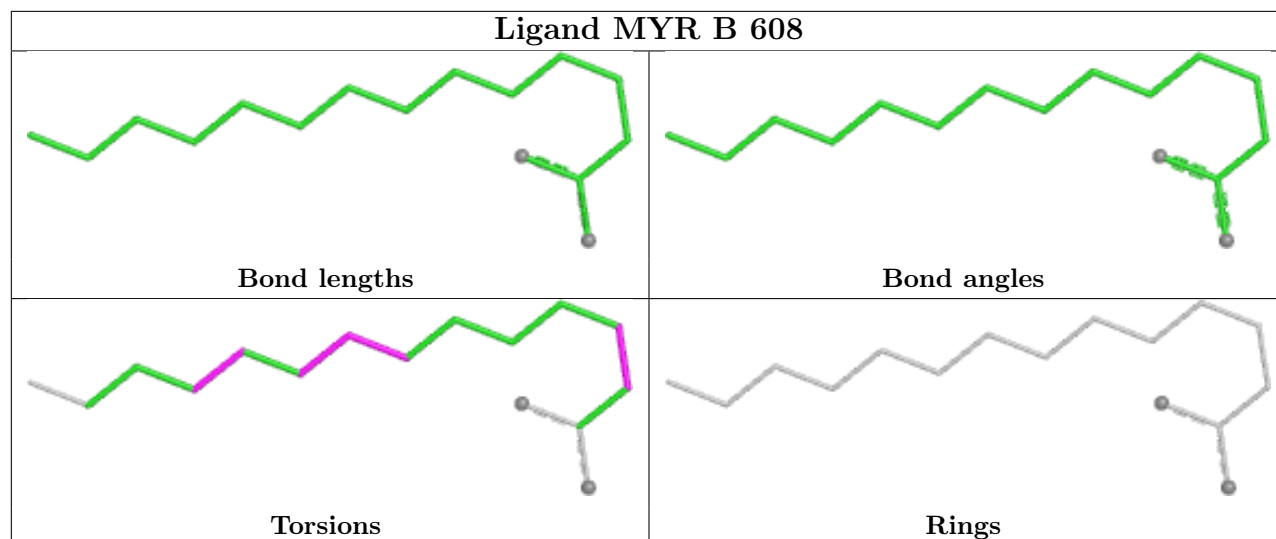
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

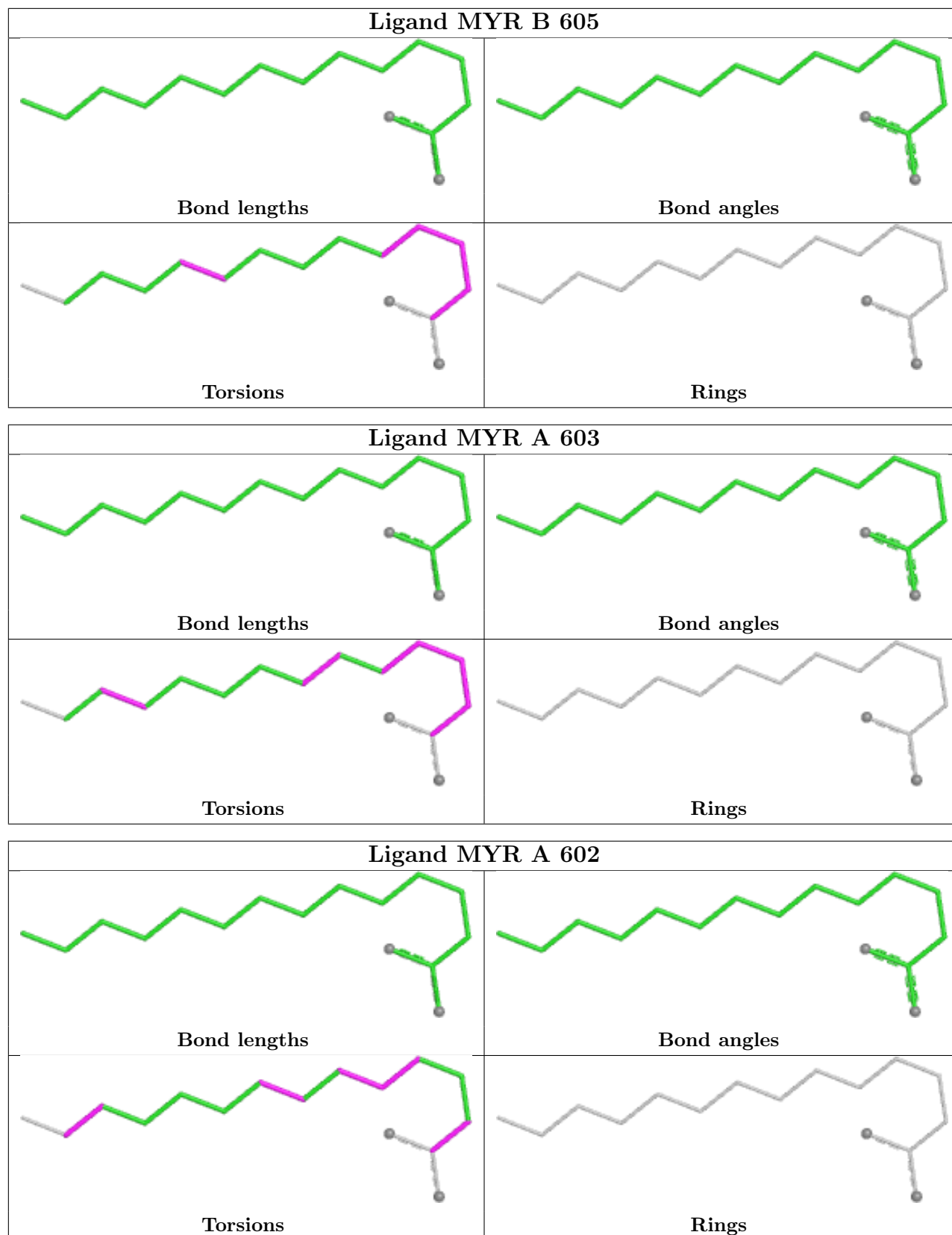












5.7 Other polymers [i](#)

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%)	0.68	45 (7%)	19 21	23, 40, 63, 88	2 (0%)
1	B	582/609 (95%)	0.79	55 (9%)	14 14	19, 42, 65, 96	3 (0%)
All	All	1164/1218 (95%)	0.73	100 (8%)	16 17	19, 42, 64, 96	5 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	584	GLY	5.9
1	B	584	GLY	5.6
1	B	583	LEU	4.9
1	B	468	PRO	4.7
1	A	561	ALA	4.6
1	B	558	CYS	4.1
1	B	566	THR	4.1
1	A	560	LYS	4.1
1	B	561	ALA	3.9
1	A	509	PHE	3.9
1	A	568	PHE	3.7
1	A	555	VAL	3.6
1	A	567	CYS	3.6
1	B	474	THR	3.5
1	A	566	THR	3.4
1	A	452	TYR	3.4
1	A	559	CYS	3.3
1	B	116	VAL	3.3
1	B	441	PRO	3.2
1	B	568	PHE	3.2
1	A	364	ALA	3.1
1	B	540	THR	3.1
1	A	517	SER	3.1
1	B	452	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	283	LEU	3.0
1	B	539	ALA	3.0
1	A	111	ASN	3.0
1	B	390	GLN	2.9
1	B	546	ALA	2.9
1	A	502	PHE	2.9
1	A	575	LEU	2.9
1	A	569	ALA	2.8
1	A	558	CYS	2.8
1	A	396	GLU	2.8
1	B	565	GLU	2.8
1	B	559	CYS	2.8
1	B	567	CYS	2.8
1	B	582	ALA	2.7
1	A	539	ALA	2.7
1	A	301	ASP	2.6
1	B	517	SER	2.6
1	B	497	TYR	2.6
1	B	514	CYS	2.6
1	A	565	GLU	2.6
1	A	202	SER	2.5
1	B	509	PHE	2.5
1	B	511	ALA	2.5
1	B	469	VAL	2.5
1	B	555	VAL	2.5
1	B	503	ASN	2.4
1	B	440	HIS	2.4
1	A	582	ALA	2.4
1	B	556	GLU	2.4
1	B	394	LEU	2.4
1	B	462	VAL	2.4
1	B	493	VAL	2.4
1	B	498	VAL	2.4
1	B	149	PHE	2.4
1	A	443	ALA	2.4
1	B	409	VAL	2.4
1	B	301	ASP	2.3
1	A	583	LEU	2.3
1	A	504	ALA	2.3
1	B	364	ALA	2.3
1	B	492[A]	GLU	2.3
1	A	390	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	516	LEU	2.3
1	B	416	PRO	2.3
1	B	475	LYS	2.3
1	B	398	LEU	2.3
1	A	468	PRO	2.3
1	A	562	ASP	2.3
1	B	396	GLU	2.3
1	A	474	THR	2.3
1	B	569	ALA	2.2
1	A	564	LYS	2.2
1	A	573	LYS	2.2
1	A	578	ALA	2.2
1	B	513	ILE	2.2
1	B	563	ASP	2.2
1	A	300	ALA	2.2
1	B	535	HIS	2.1
1	A	554	PHE	2.1
1	B	502	PHE	2.1
1	A	30	TYR	2.1
1	A	513	ILE	2.1
1	A	467	THR	2.1
1	B	434	GLY	2.1
1	B	463	LEU	2.1
1	B	553	ALA	2.1
1	B	435	SER	2.1
1	A	204	GLN	2.1
1	A	501	GLU	2.0
1	A	306	ALA	2.0
1	A	581	ALA	2.0
1	B	362	ALA	2.0
1	A	439	LYS	2.0
1	B	202	SER	2.0
1	A	367	HIS	2.0
1	A	510	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

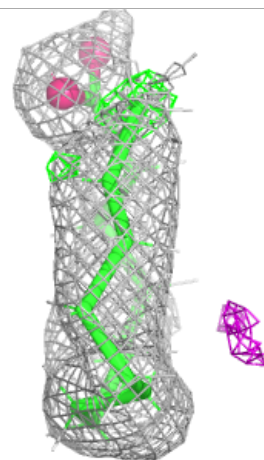
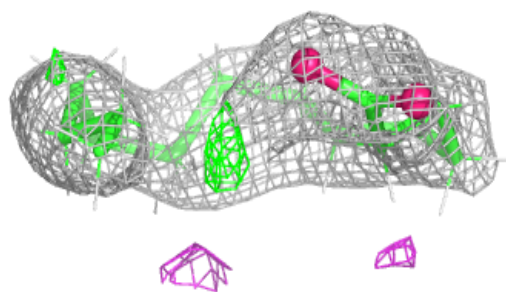
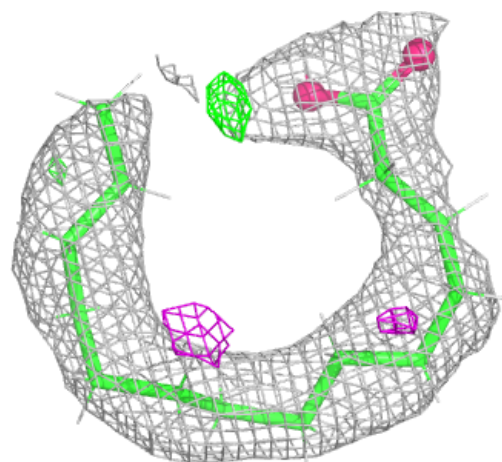
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MYR	B	607	16/16	0.82	0.16	37,51,66,69	0
2	MYR	A	604	16/16	0.83	0.16	38,53,69,69	0
2	MYR	B	608	16/16	0.83	0.16	39,52,62,69	44
2	MYR	B	604	16/16	0.84	0.16	39,55,67,76	0
2	MYR	A	608	16/16	0.84	0.16	34,49,61,68	44
2	MYR	B	601	16/16	0.84	0.16	29,47,63,76	44
2	MYR	A	601	16/16	0.86	0.15	35,50,61,64	0
2	MYR	A	607	16/16	0.86	0.14	27,52,67,77	0
2	MYR	B	602	16/16	0.86	0.16	29,50,67,67	0
2	MYR	A	606	16/16	0.87	0.13	23,44,57,60	0
2	MYR	B	605	16/16	0.87	0.12	40,54,65,82	0
2	MYR	A	605	16/16	0.88	0.12	30,54,65,69	0
2	MYR	B	606	16/16	0.88	0.14	30,46,58,66	0
2	MYR	B	603	16/16	0.89	0.15	27,51,66,69	0
2	MYR	A	602	16/16	0.89	0.13	26,49,75,78	0
3	EDO	B	609	4/4	0.90	0.14	33,42,55,64	0
2	MYR	A	603	16/16	0.92	0.12	19,46,58,62	0
3	EDO	A	609	4/4	0.95	0.07	33,39,46,48	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.

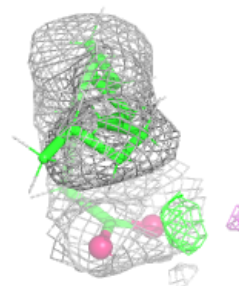
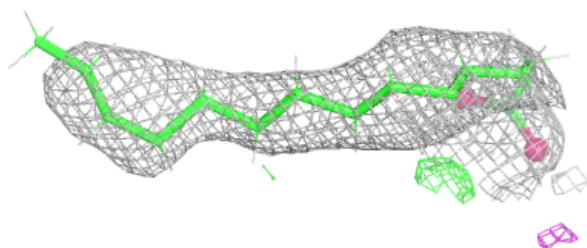
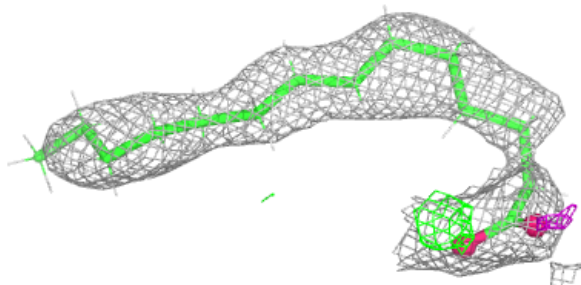
Electron density around MYR B 607:

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

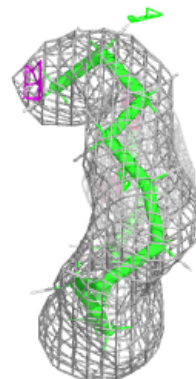
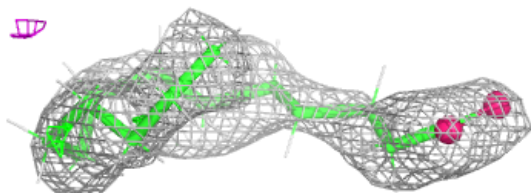


Electron density around MYR A 604:

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

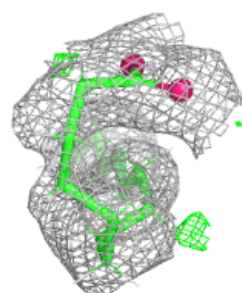
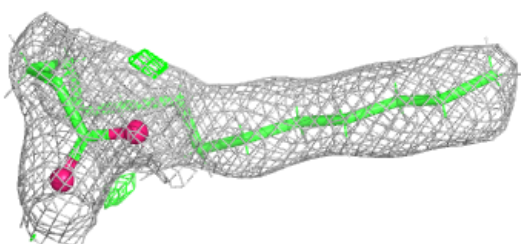
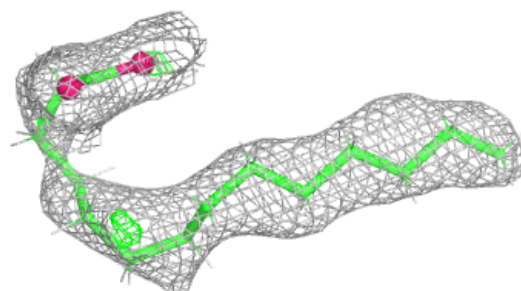
**Electron density around MYR B 608:**

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

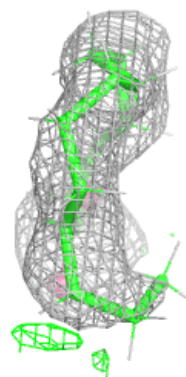
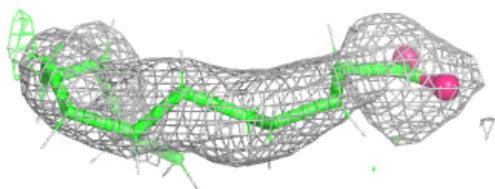
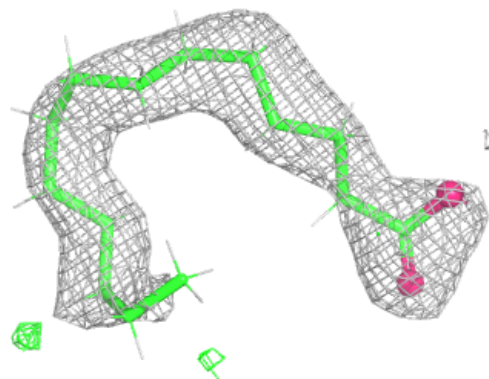


Electron density around MYR B 604:

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

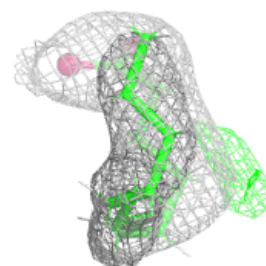
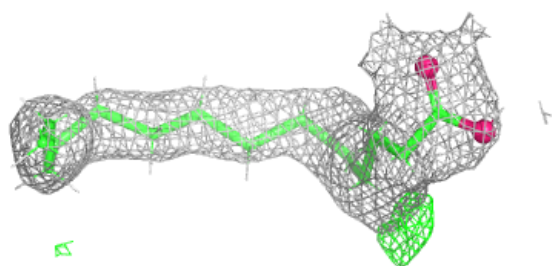
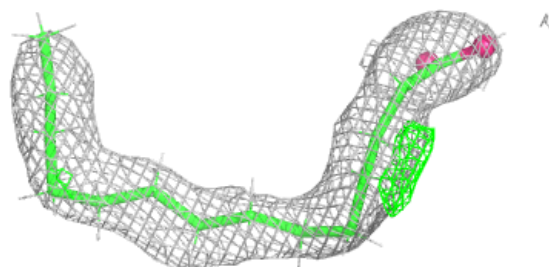
**Electron density around MYR A 608:**

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

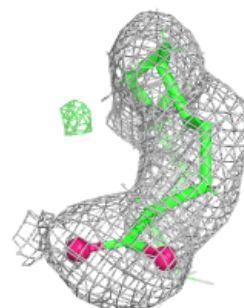
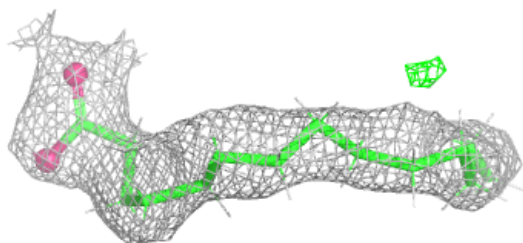
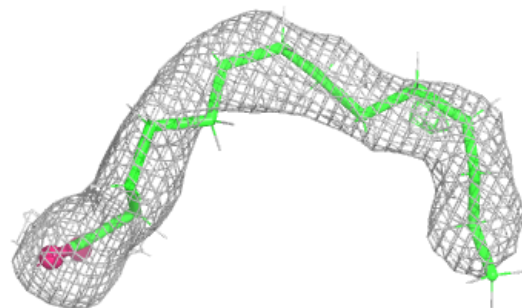


Electron density around MYR B 601:

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

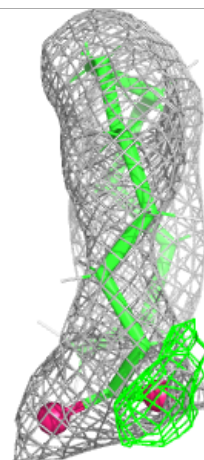
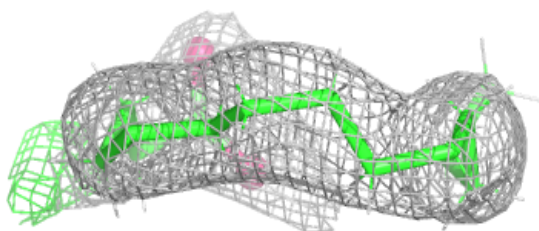
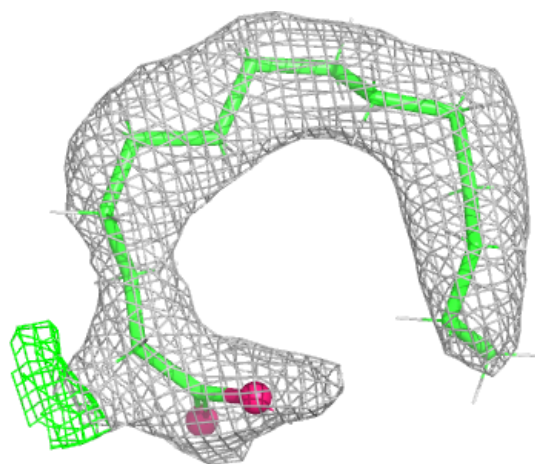
**Electron density around MYR A 601:**

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



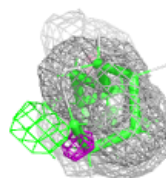
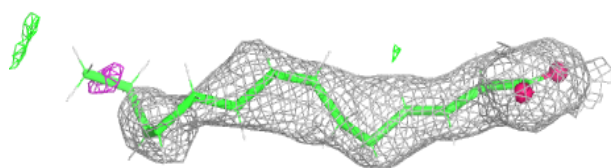
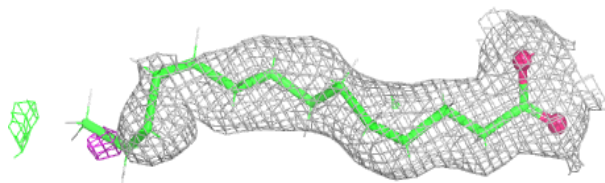
Electron density around MYR A 607:

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

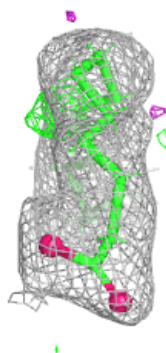
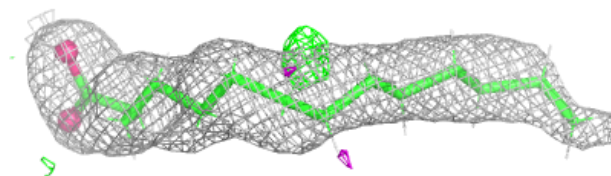
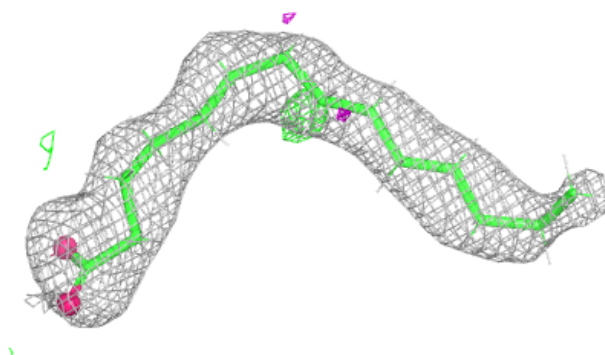


Electron density around MYR B 602:

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

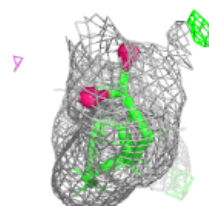
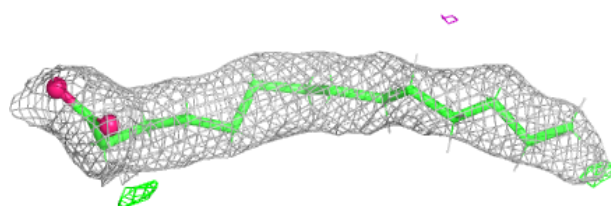
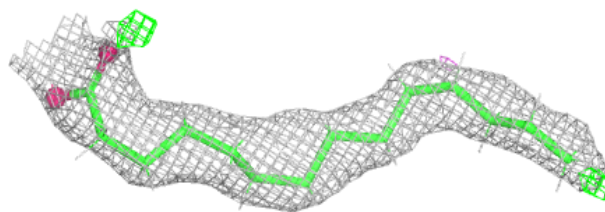
**Electron density around MYR A 606:**

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

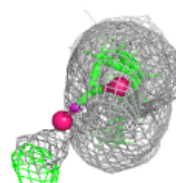
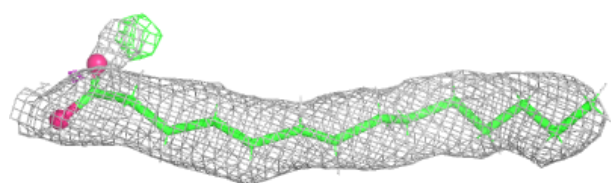
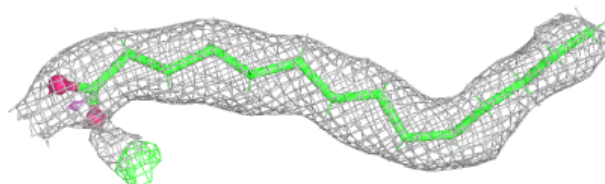


Electron density around MYR B 605:

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

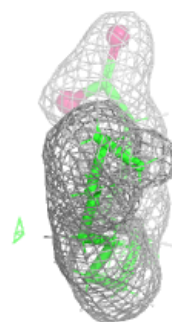
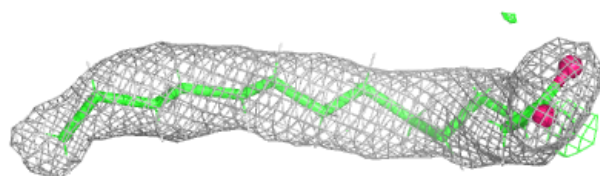
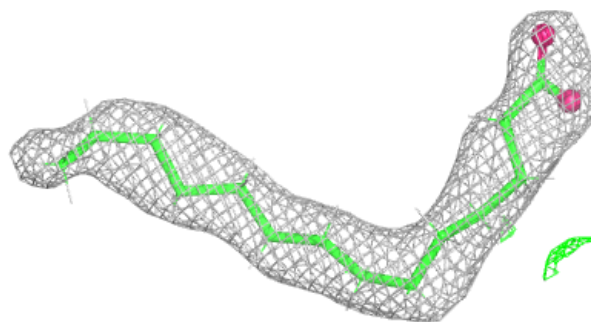
**Electron density around MYR A 605:**

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

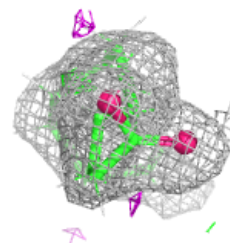
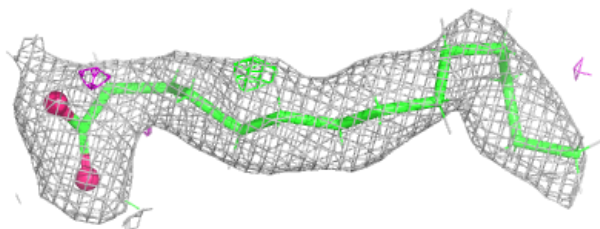
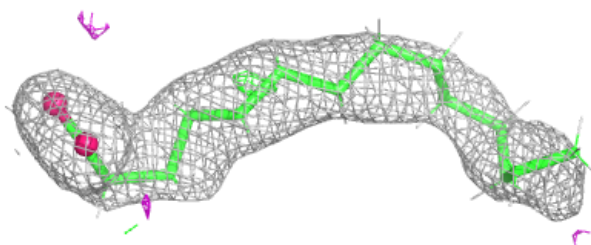


Electron density around MYR B 606:

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

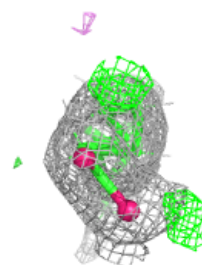
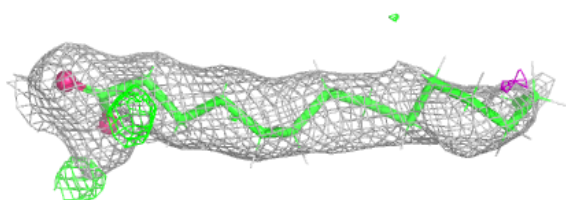
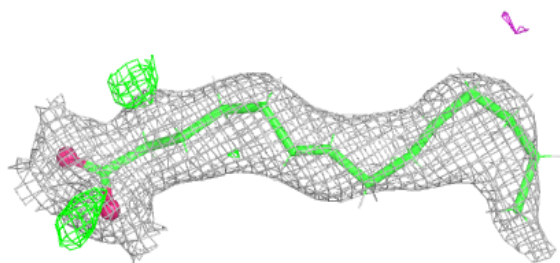
**Electron density around MYR B 603:**

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

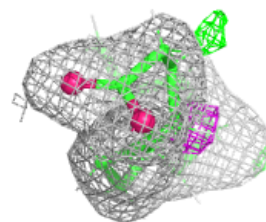
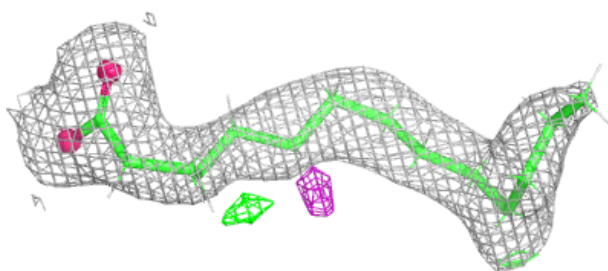
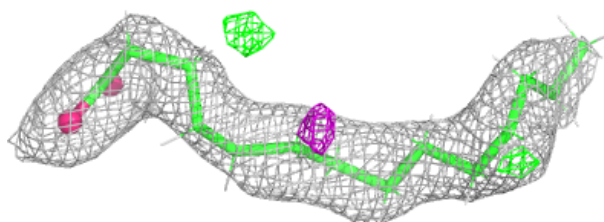


Electron density around MYR A 602:

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

**Electron density around MYR A 603:**

$2mF_o-DF_c$ (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.